

Learning with differentiable and amortized optimization

Brandon Amos • Meta AI (FAIR)



github.com/facebookresearch/presentations

Optimization is crucial technology

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

Breakthroughs over the past century enabled by optimization advancements 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
for **optimal transport** and **generative modeling**
4. **allocating** budgets and portfolios,
5. **designing** materials, molecules, and other structures,
6. **solving inverse problems**
infers underlying hidden costs, incentives, geometries, terrains, and other structures
7. **parameter learning** of predictive and statistical models

Optimal control drives systems

Setting: deterministic, discrete-time system with a **continuous state-action space**

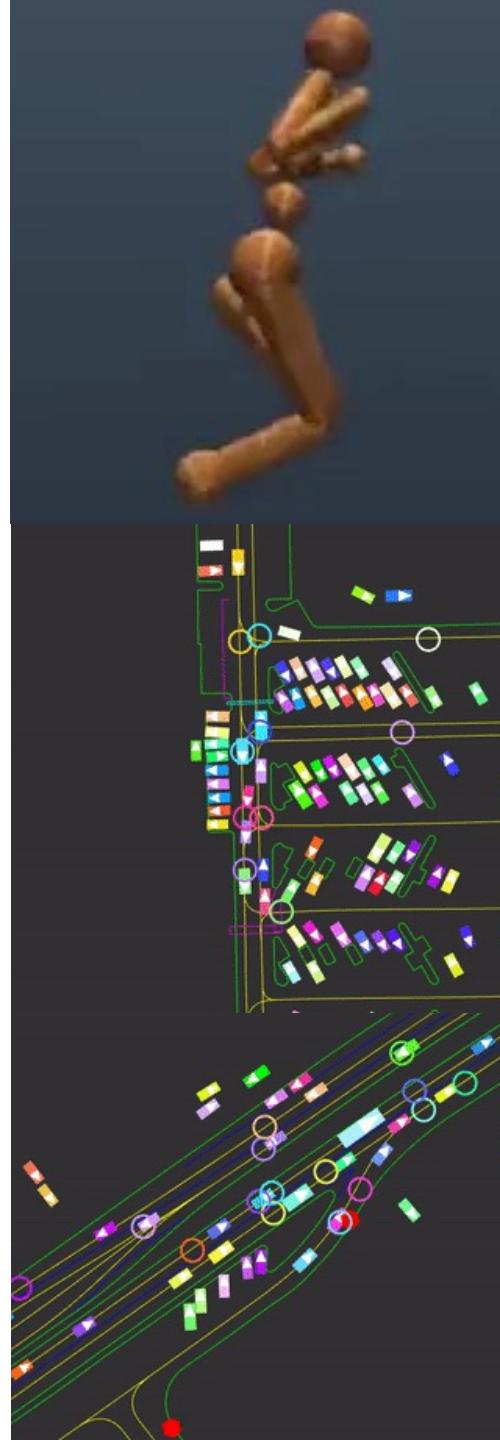
$$x_{1:T}^*, u_{1:T}^* \in \operatorname{argmin}_{x_{1:T}, u_{1:T}} \sum_t \begin{array}{|c|} \text{cost} \\ \hline C_\theta(x_t, u_t) \end{array} \text{ s.t. } \begin{array}{|c|} \text{initial state} \\ \hline x_1 = x_{\text{init}} \end{array} \quad \begin{array}{|c|} \text{dynamics} \\ \hline x_{t+1} = f_\theta(x_t, u_t) \end{array} \quad \begin{array}{|c|} \text{constraints} \\ \hline u_t \in \mathcal{U} \end{array}$$

Full notation: $u_{1:T}^*(x_{\text{init}}, f_\theta)$

Widely deployed over the past century in aviation, robotics, vehicles, HVAC
Often for a **Markov decision process** but doesn't have to be

The **real-world is non-convex**, so are our controllers
Convex in some cases, e.g., with quadratic cost/linear dynamics (LQR)

No learning necessary if we know the system — just pure optimization



Optimal transport connects measures

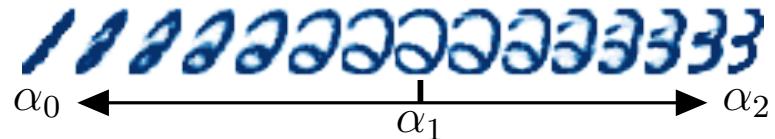
Setting: transport between measures α and β

Monge problem for Euclidean Wasserstein-2

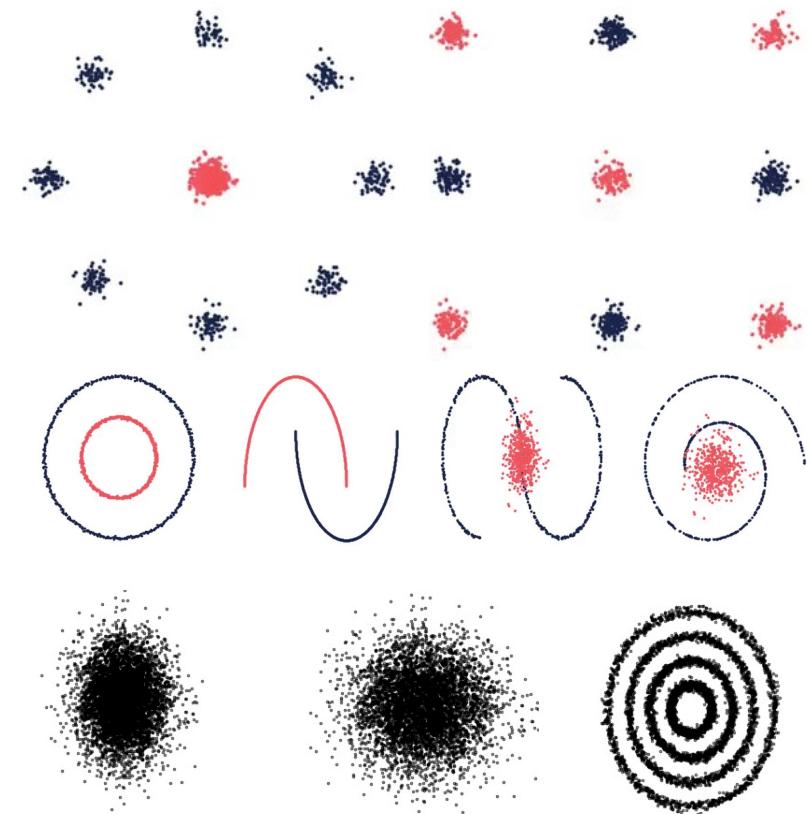
$$T^*(\alpha, \beta) \in \operatorname{argmin}_{T \in \mathcal{C}(\alpha, \beta)} \mathbb{E}_{x \sim \alpha} \|x - T(x)\|_2^2$$

The transport map T^* **connects** α to β

No learning necessary, again just optimization



Meta Optimal Transport. Amos et al., 2022

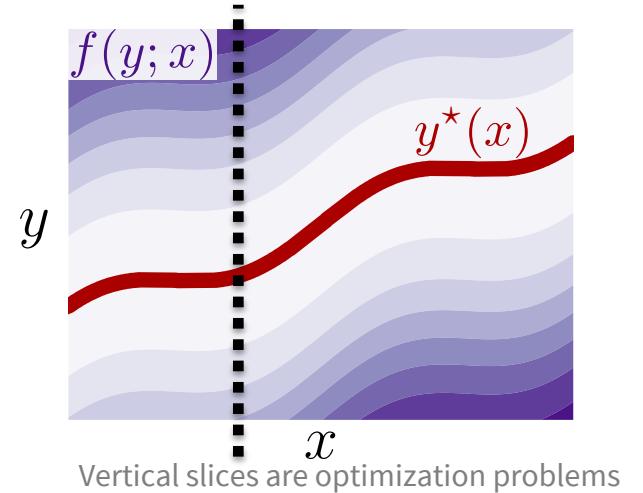


On amortizing convex conjugates for optimal transport. Amos, 2022

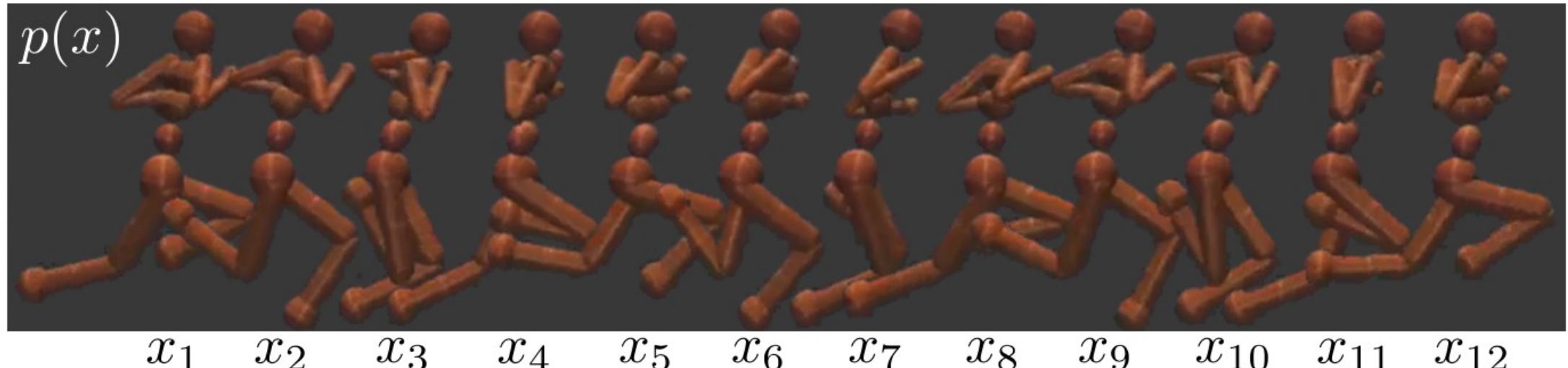
The magic of optimization

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

$$\begin{array}{c} \text{optimal solution} \\ | \\ y^*(x) \in \operatorname{argmin}_{y \in \mathcal{C}(x)} f(y; x) \\ | \qquad \qquad \qquad | \\ \text{optimization variable} \quad \text{constraints} \\ | \qquad \qquad \qquad | \\ \text{objective} \qquad \text{context (or parameterization)} \end{array}$$



In control, x is the **system state**, y is the **action**, $f(y; x)$ is a **cost**, and $y^*(x)$ is an **optimal action**



When optimization fails, machine learning helps

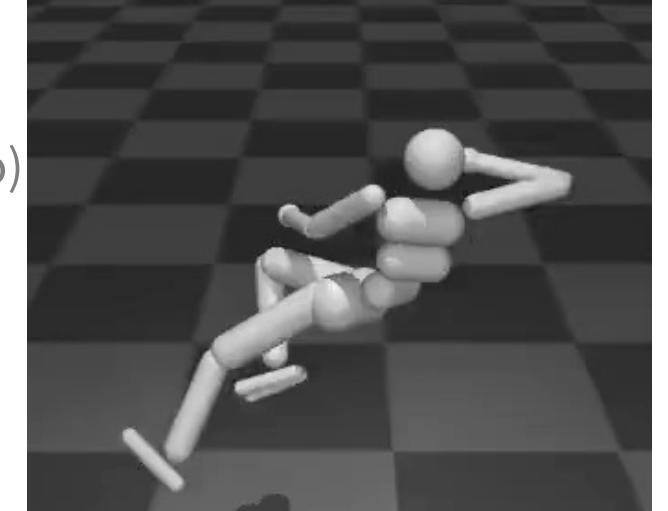
$$y^*(x) \in \operatorname{argmin}_{y \in \mathcal{C}(x)} f(y; x)$$

Optimization starts failing us when:

1. Analytically **encoding every detail** into f and \mathcal{C} is impossible
 - May be **unknown, mis-specified, or inaccurate**
 - Especially difficult with **high-dimensional data** (text, images, video)
2. **Solving** for $y^*(x)$ is **intractable** and **difficult to compute**

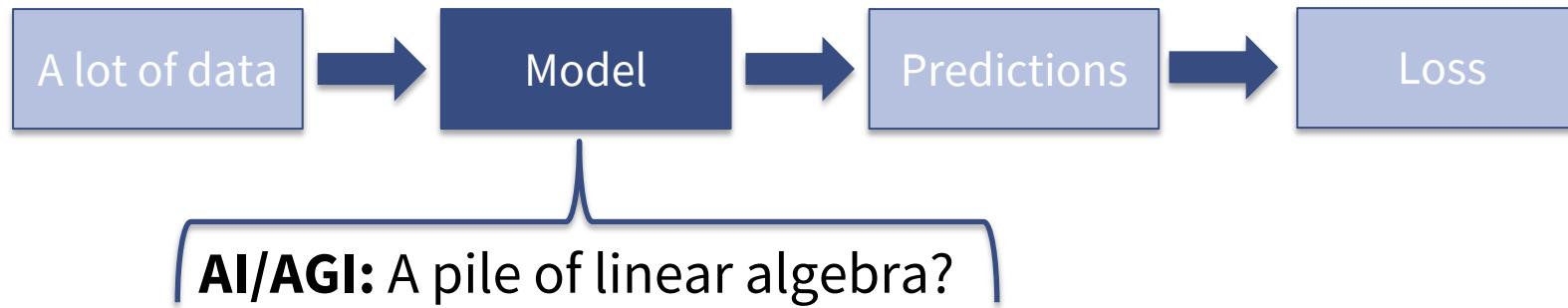
Machine learning systems are **part of the solution** and **excel** at:

1. **Modeling systems** we can extract a lot of data from
2. Extracting **meaningful latent representations**
3. Making **fast and accurate** predictions



When optimization fails, machine learning helps

When machine learning fails, optimization helps

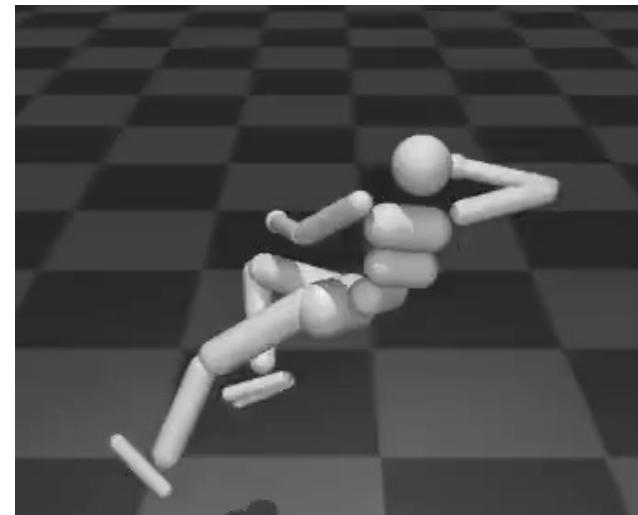


Is a **black-box of linear algebra** the **solution to AI/AGI?** *Maybe...*

Without enough data, learning systems struggle to:

1. **Encode hard constraints** and **rules** of the world crucial for safety
2. Perform **reasoning operations**
3. Isolate **interpretable** and **modular subcomponents**
4. **Generalize** to new settings beyond the training distribution

Optimization often **excels in these** and **can be brought into the model/loss**



Integrating optimization and machine learning

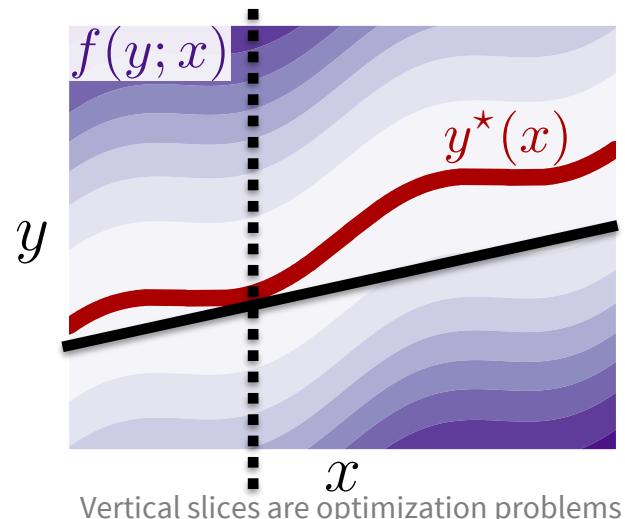
Key: view **optimization as a function** from the context x to the solution $y^*(x) \in \operatorname{argmin}_{y \in \mathcal{C}(x)} f(y; x)$

Differentiable optimization — $\frac{\partial}{\partial x} y^*(x)$

Optimization is just a function that can be *differentiated*

Tells how **perturbing the context changes the solution**

Enables **optimization as a layer** or loss for ML

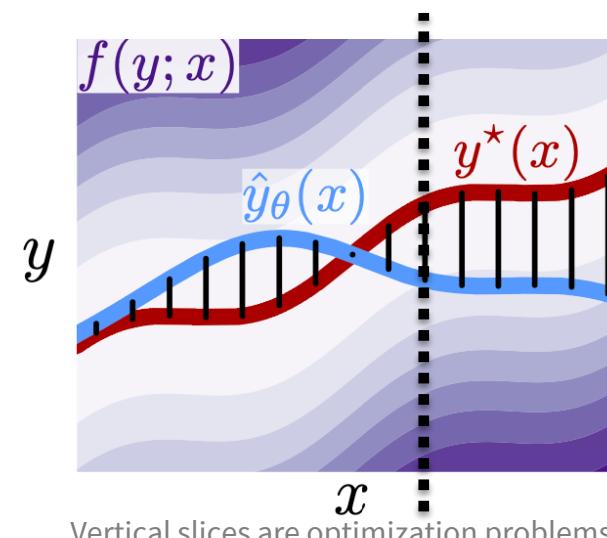


Amortized optimization — $\hat{y}_\theta(x) \approx y^*(x)$

Optimization is just a function that can be *approximated*

Approximate the solution map with \hat{y}_θ

Power of optimization, fast speed of an ML model



This talk

Differentiable optimization — $\frac{\partial}{\partial x} y^*(x)$

Foundations

Differentiable convex optimization layers

Differentiable control

Optimization-based task losses

Amortized optimization — $\hat{y}_\theta(x) \approx y^*(x)$

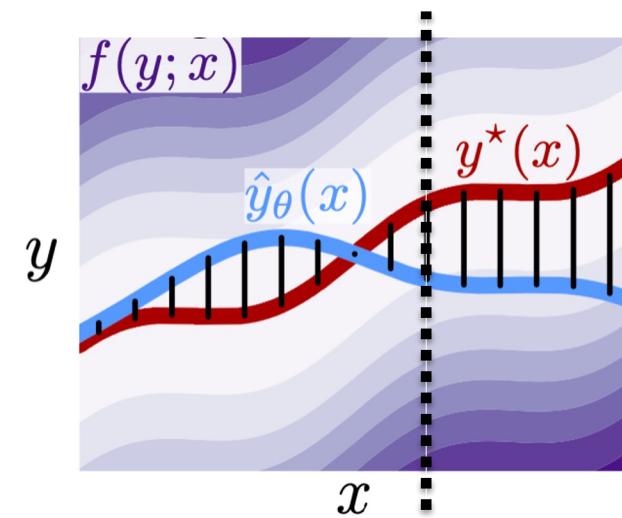
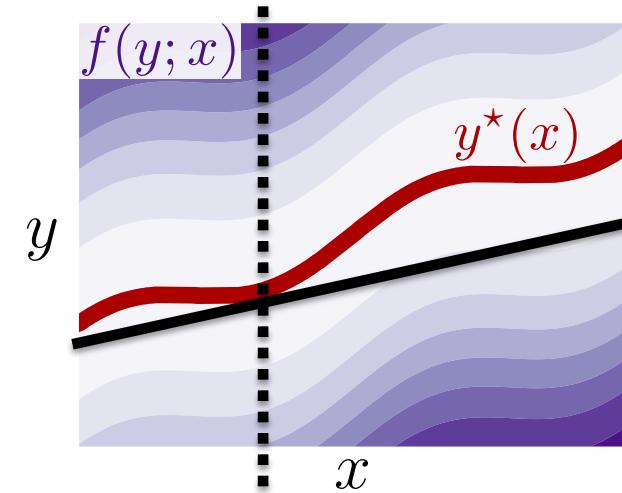
Foundations

RL as amortized optimization

Amortization via learning latent subspaces

Meta Optimal Transport

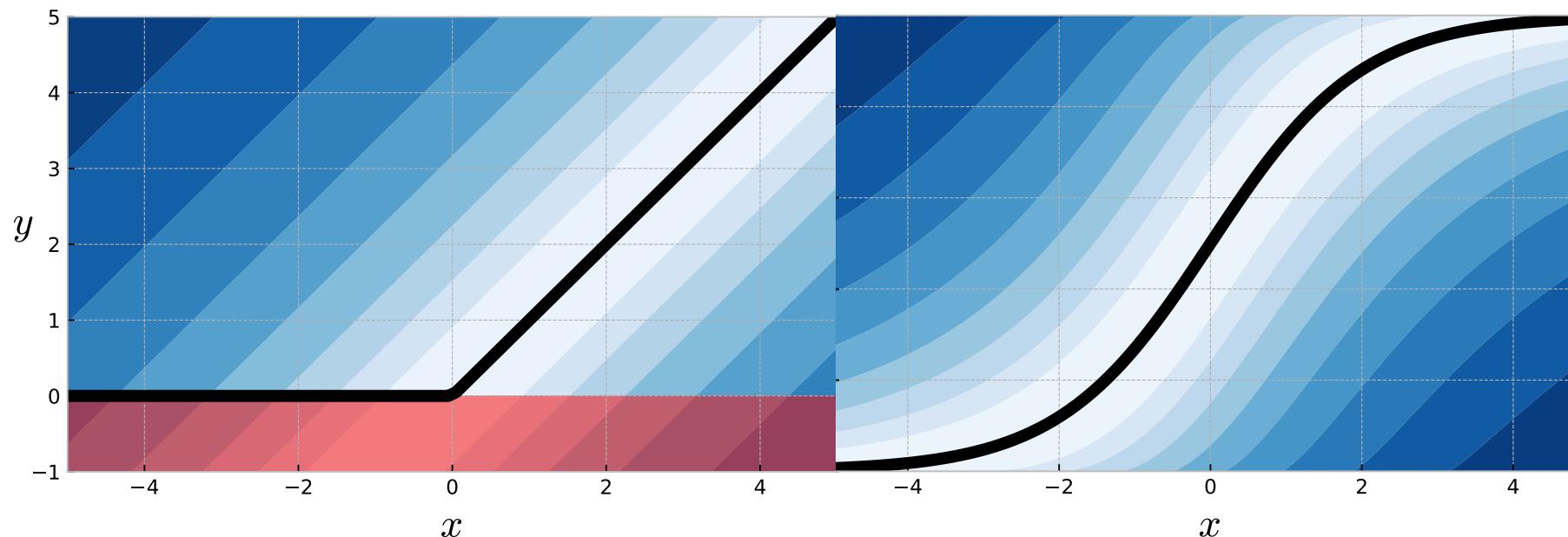
Amortizing convex conjugates



Convex optimization is expressive

The **argmin** of a **convex** optimization problem is **non-convex** and **expressive**
Standard non-linearities to be seen as **solutions** to convex optimization problems
We'll start simple for **intuition** and **motivation to generalize beyond these**

$$y^*(x) = \underset{y}{\operatorname{argmin}} f(y; x) \text{ subject to } y \in C(x)$$

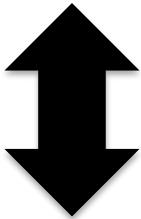


The ReLU is a convex optimization layer

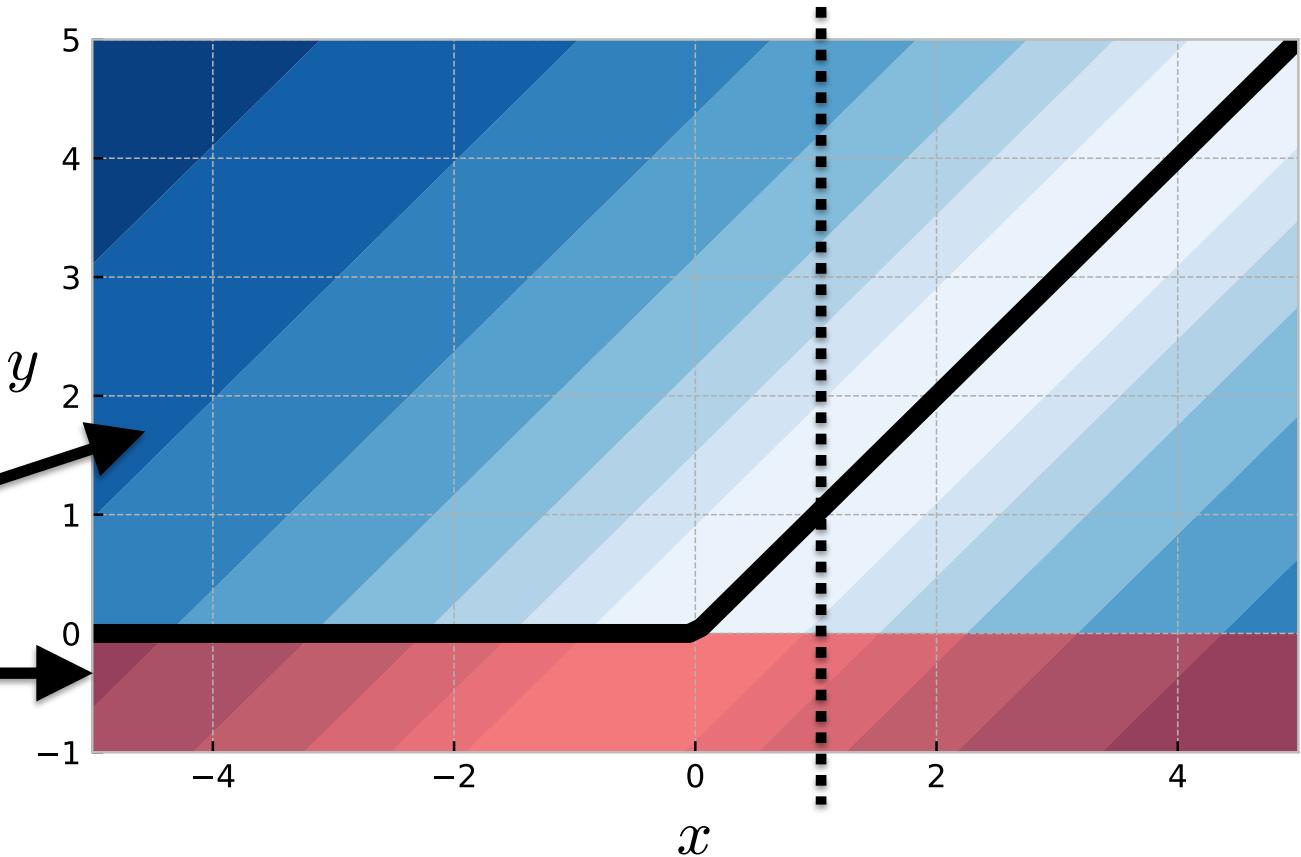
Section 2 of Differentiable optimization-based modeling for machine learning. Amos, PhD Thesis 2019

Proof: Comes from first-order optimality

$$\text{ReLU}(x) = \max\{0, x\}$$



$$\begin{aligned} \text{ReLU}(x) &= \operatorname{argmin}_y \|y - x\|_2^2 \\ \text{s.t. } y &\geq 0 \end{aligned}$$

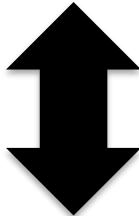


The sigmoid is a convex optimization layer

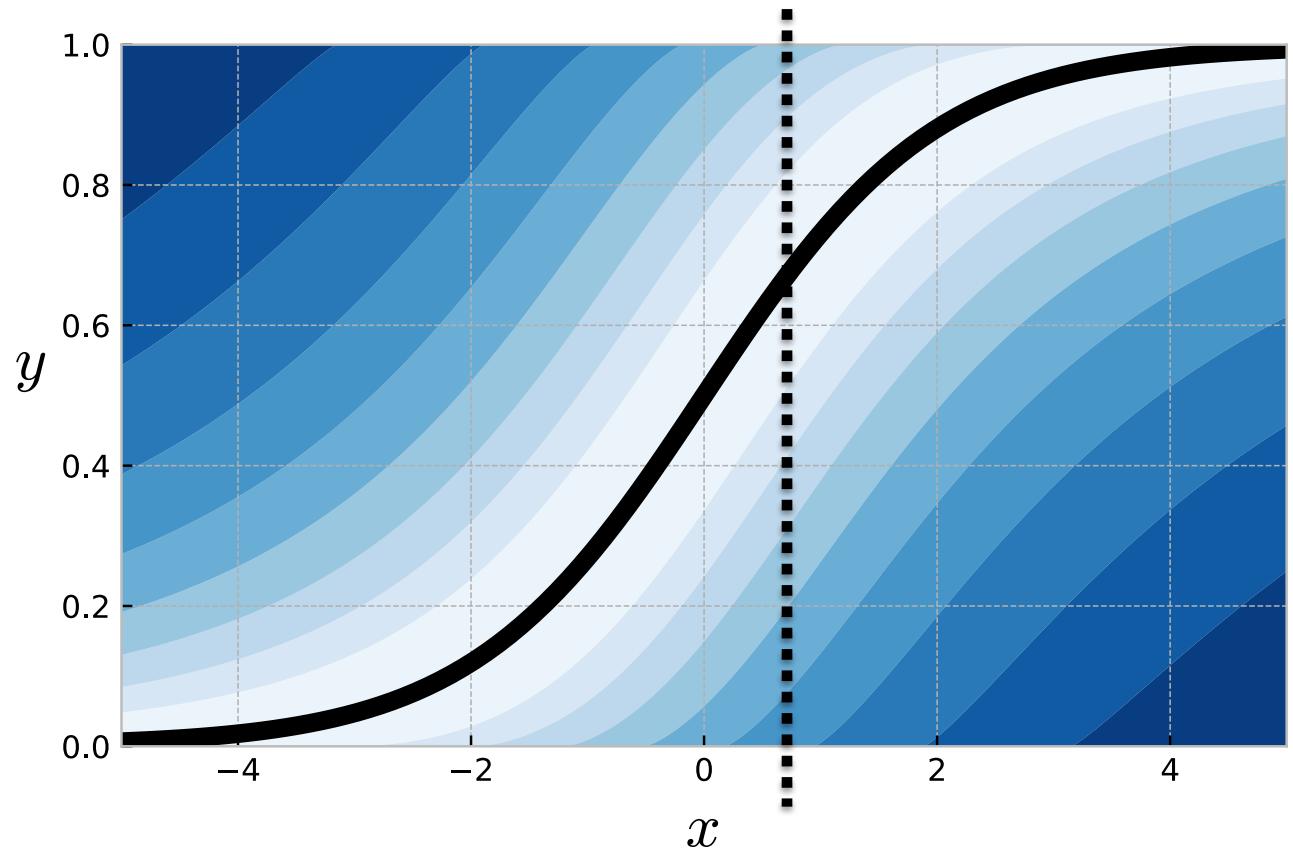
Section 2 of Differentiable optimization-based modeling for machine learning. Amos, PhD Thesis 2019

Proof: Comes from first-order optimality

$$\sigma(x) = \frac{1}{1 + \exp \{-x\}}$$



$$\begin{aligned} \sigma(x) = \operatorname{argmin}_y & -y^T x - H_b(y) \\ \text{s.t. } & 0 \leq y \leq 1 \end{aligned}$$



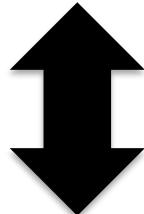
$H_b(y) := -\sum_i(y_i \log y_i + (1 - y_i) \log(1 - y_i))$ is the binary cross-entropy function

The softargmax is a convex optimization layer

Section 2 of *Differentiable optimization-based modeling for machine learning*. Amos, PhD Thesis 2019

Proof: Comes from first-order optimality

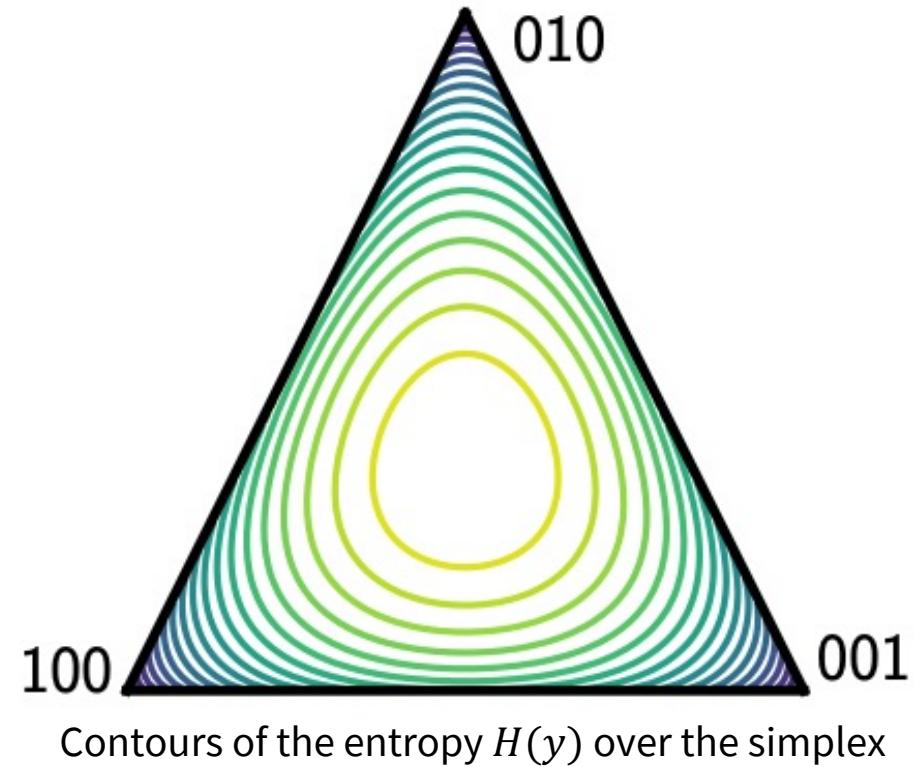
$$\pi_{\Delta}(x) = \frac{\exp x}{\sum_i \exp x_i}$$



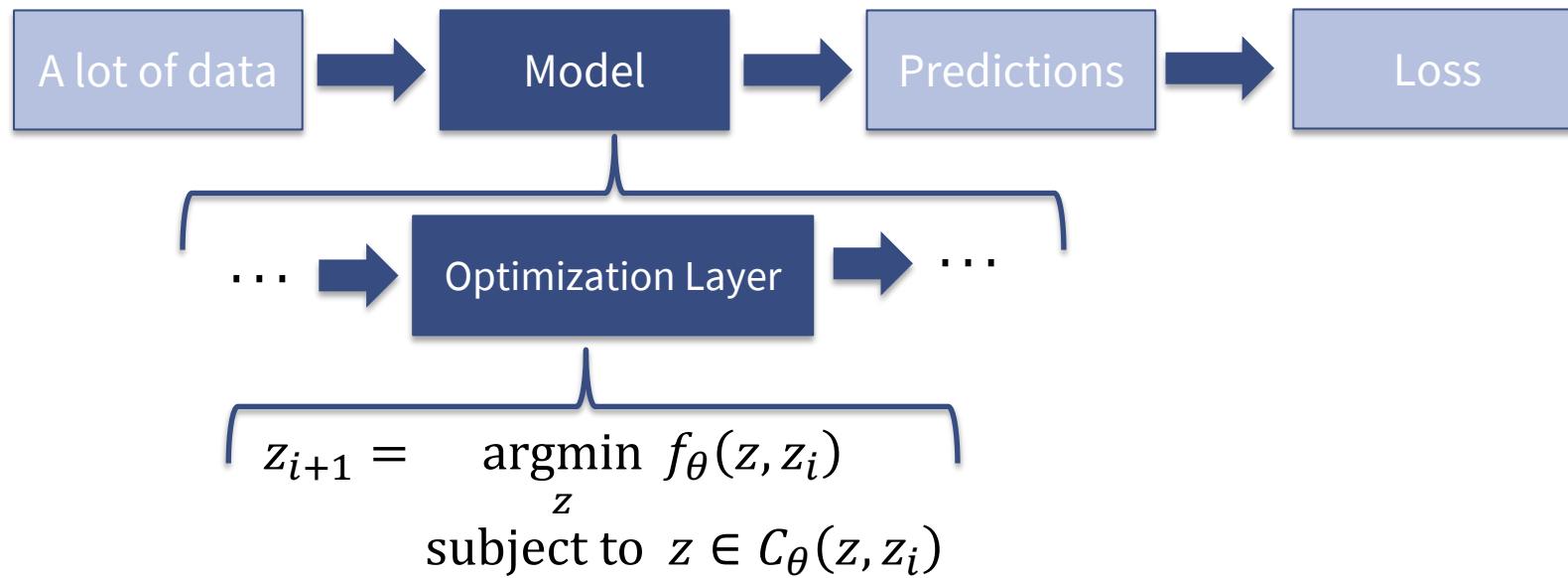
$$\pi_{\Delta}(x) = \operatorname{argmin}_y -y^T x - H(y)$$

$$\begin{aligned} \text{s.t. } & 0 \leq y \leq 1 \\ & 1^T y = 1 \end{aligned}$$

$H(y) := -\sum_i y_i \log y_i$ is the entropy function



How can we generalize this?



Derivatives and backpropagation

For learning, we **differentiate** or backpropagate through these layers — **differentiable optimization**

Easy if the optimization problem has an **explicit, closed-form solution** (often standard differentiation)

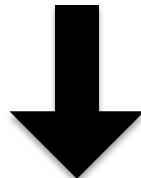
Otherwise, need to use **implicit differentiation**, which is also used for sensitivity analysis

Differentiable convex quadratic programs

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

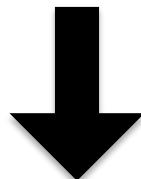
$$x^* = \underset{x}{\operatorname{argmin}} \frac{1}{2} x^\top Q x + p^\top x$$

subject to $Ax = b$ $Gx \leq h$



KKT Optimality

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



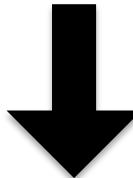
Implicitly differentiating \mathcal{R} gives $D_\theta(z^*) = -\left(D_z \mathcal{R}(z^*)\right)^{-1} D_\theta \mathcal{R}(z^*)$

Differentiable convex conic programs

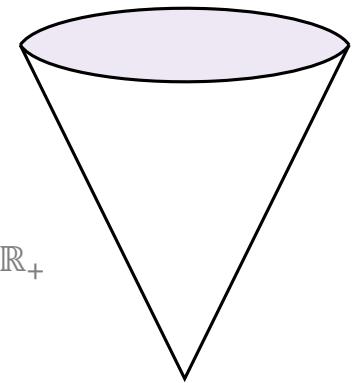
Section 7 of Differentiable optimization-based modeling for machine learning. Amos, PhD Thesis 2019
Differentiating through a cone program. Agrawal et al., 2019

$$x^* = \underset{x}{\operatorname{argmin}} \ c^T x$$

subject to $b - Ax \in \mathcal{K}$

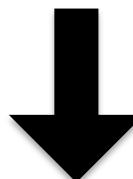


- Zero: $\{0\}$
- Free: \mathbb{R}^n
- Non-negative: \mathbb{R}_+^n
- Second-order (Lorentz): $\{(t, x) \in \mathbb{R}_+ \times \mathbb{R}^n | \|x\|_2 \leq t\}$
- Semidefinite: \mathbb{S}_+^n
- Exponential: $\{(x, y, z) \in \mathbb{R}^3 | ye^{x/y} \leq z, y > 0\} \cup \mathbb{R}_- \times \{0\} \times \mathbb{R}_+$
- Cartesian Products: $\mathcal{K} = \mathcal{K}_1 \times \dots \times \mathcal{K}_p$



Conic Optimality

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



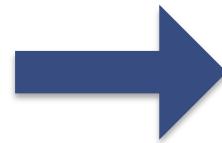
Implicitly differentiating \mathcal{R} gives $D_\theta(z^*) = -(D_z \mathcal{R}(z^*))^{-1} D_\theta \mathcal{R}(z^*)$

From the softmax to soft and differentiable top-k

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

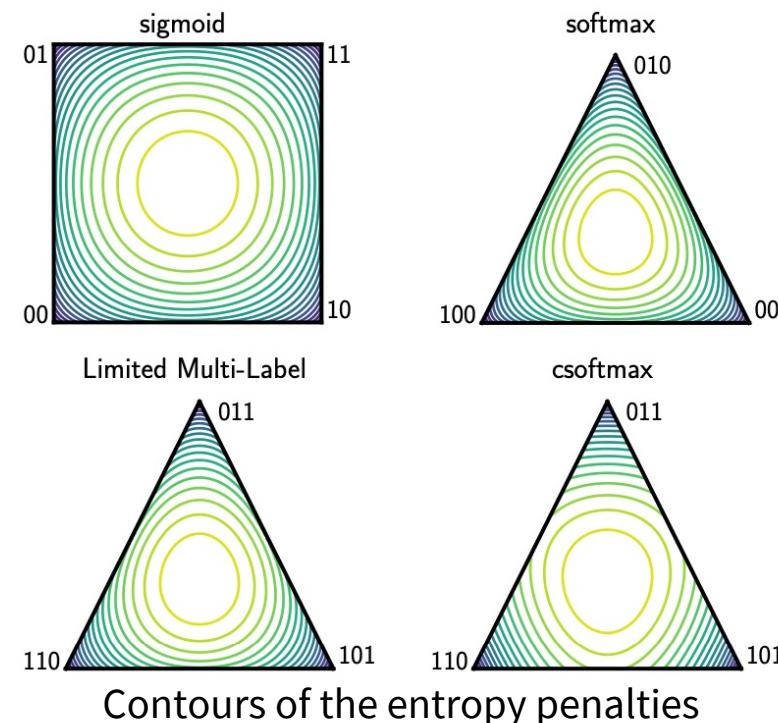
$$y^* = \underset{y}{\operatorname{argmin}} -y^\top x - H(y)$$

subject to $0 \leq y \leq 1$
 $1^\top y = \boxed{1}$

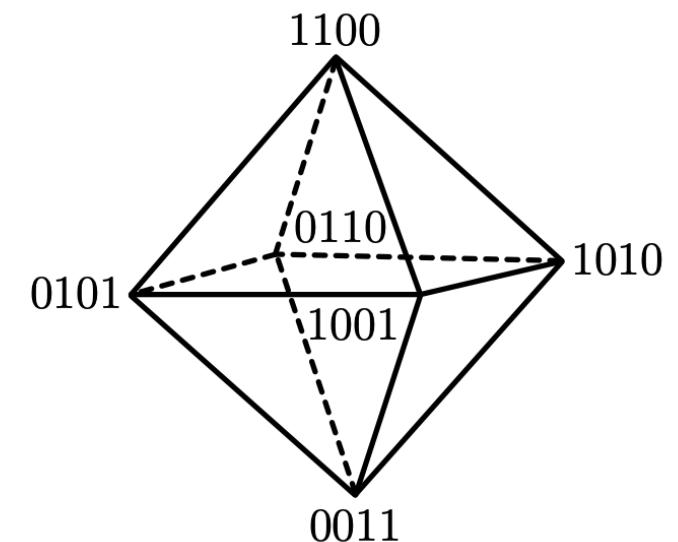
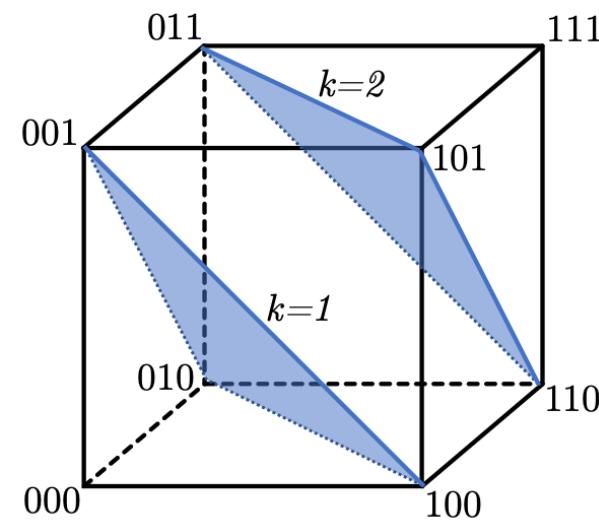


$$y^* = \underset{y}{\operatorname{argmin}} -y^\top x - H_b(y)$$

subject to $0 \leq y \leq 1$
 $1^\top y = \boxed{k}$



$H_b(y) := -\sum_i(y_i \log y_i + (1 - y_i) \log(1 - y_i))$ is the binary cross-entropy function



Differentiable permutations, sorting and SVMs

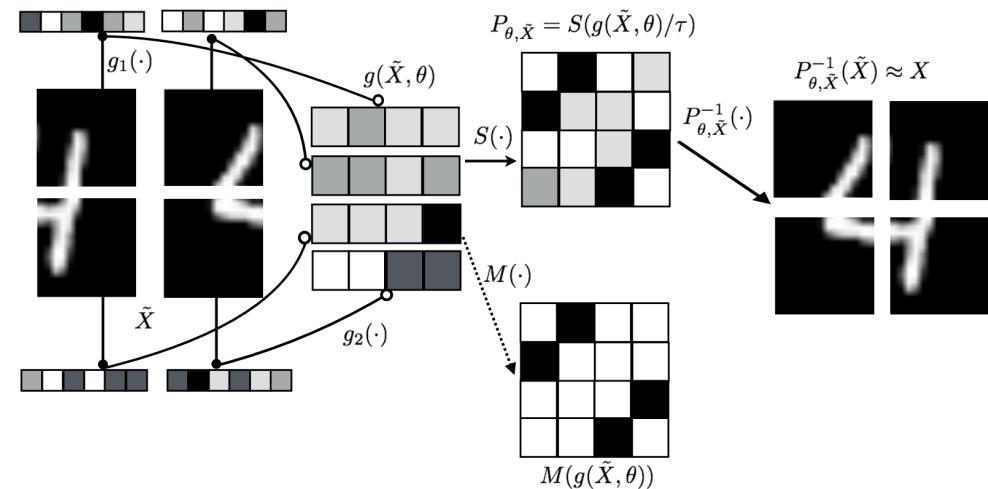
Differentiable permutations and sorting (Gumbel-Sinkhorn)

Projection onto the **Birkhoff polytope** \mathcal{B}_N :

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

$$\mathcal{B}_N = \{X: X \geq 0, \sum_i X_{ij} = \sum_j X_{ij} = 1\}$$

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

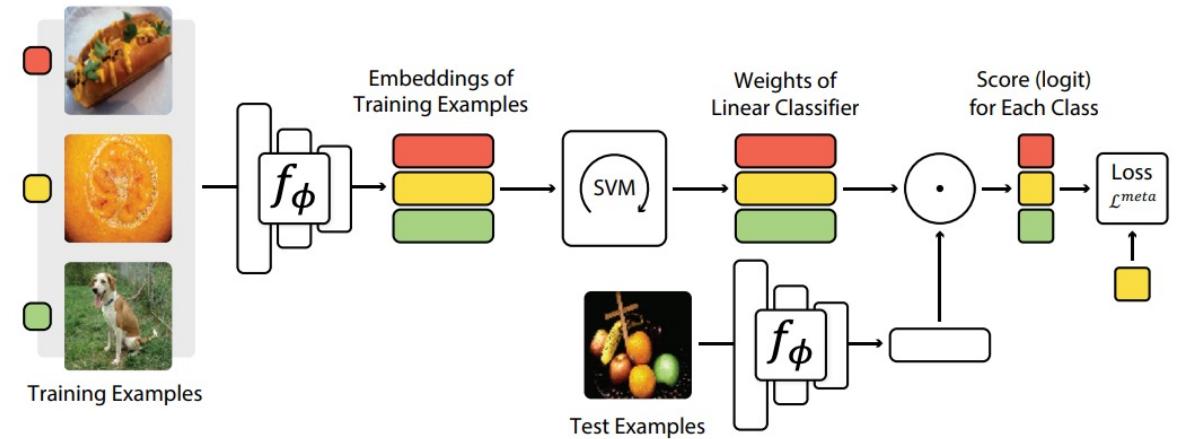


Differentiable SVMs (MetaOptNet)

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

$$w^*(\mathcal{D}) = \underset{w}{\operatorname{argmin}} \|w\|^2 + C \sum_i \max\{0, 1 - y_i f(x_i)\}$$

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



Sensitivity and perturbation analysis

Differentiable convex optimization layers. Agrawal*, Amos*, et al., NeurIPS 2019.

Adjoint derivatives for optimization problems have been studied for decades
We have focused on uses for learning, but also widely used for **sensitivity analysis**

Logistic regression example

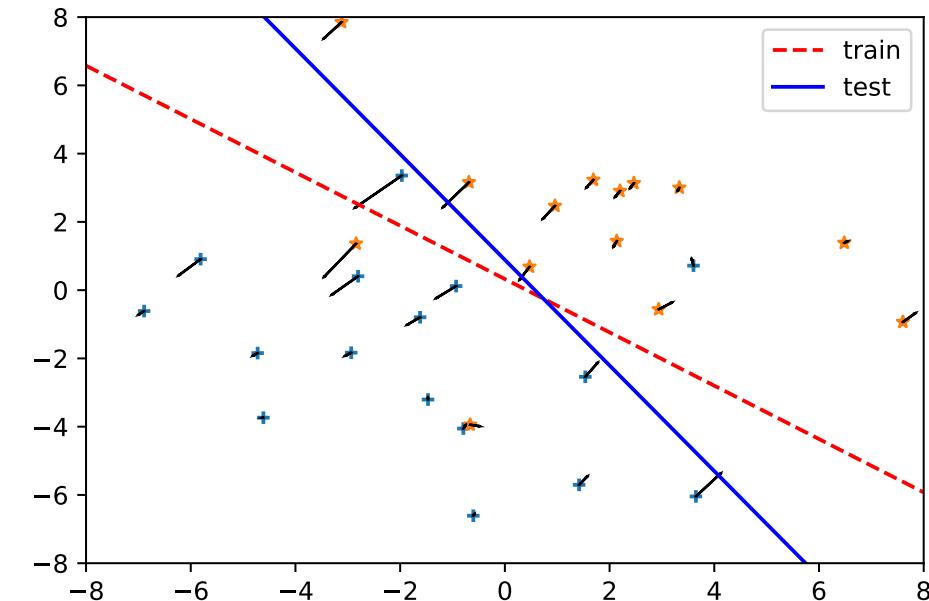
Find optimal decision boundary:

$$\theta^*(\mathcal{D}) \in \operatorname{argmax}_{\theta} \sum_i \log p_{\theta}(y_i | x_i)$$

$\theta^*(\mathcal{D})$ is **just a function** of the data

Derivatives $\frac{\partial \theta^*}{\partial x_i}$ provide **sensitivity** to the data points

- *Show how much the data impacts the decision boundary*



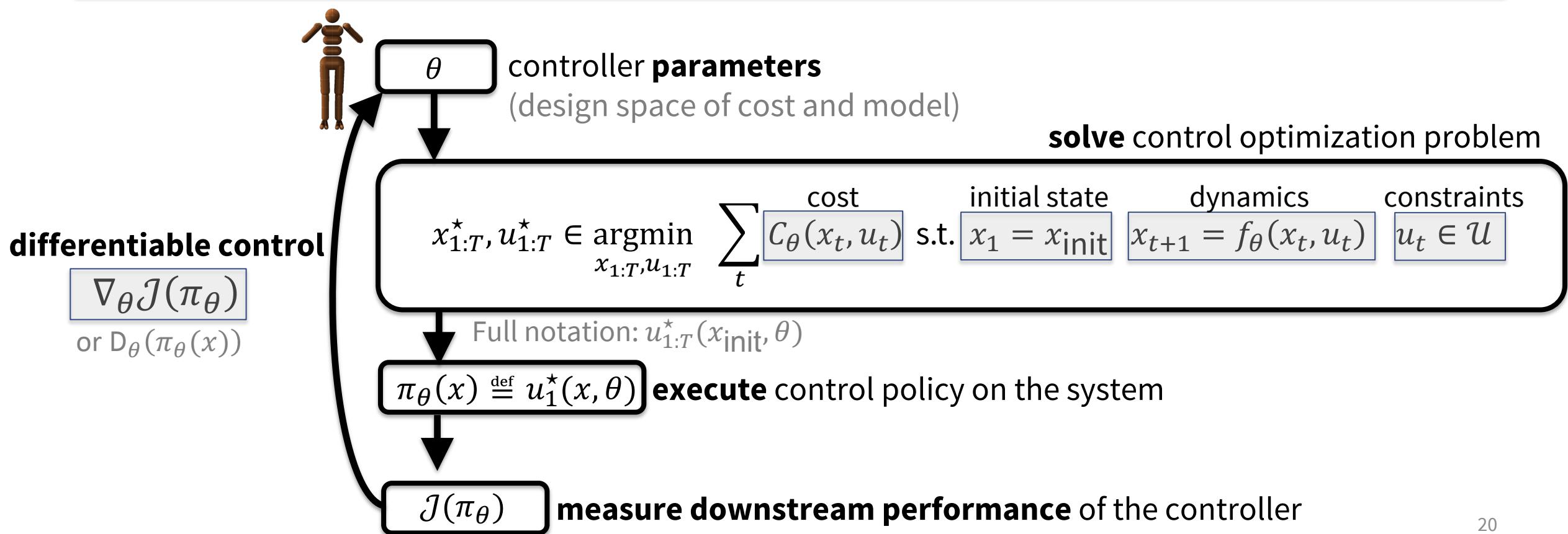
Differentiable control

Differentiable MPC for end-to-end planning and control. Amos et al., NeurIPS 2018.

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

We can often measure the **downstream performance** induced by the controller

Idea: optimize (i.e., tune/learn) the parameters for a **downstream performance metric** by **differentiating through the control optimization problem**



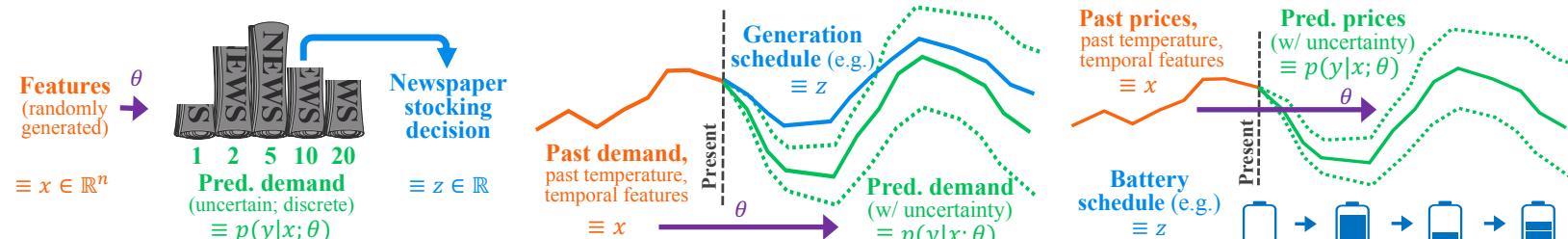
Optimization as a loss for downstream tasks

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

A model's predictions may be used in a **downstream optimization problem** (e.g., scheduling)

Challenge: models are **inaccurate** and **not aware of how errors impact the downstream problem**

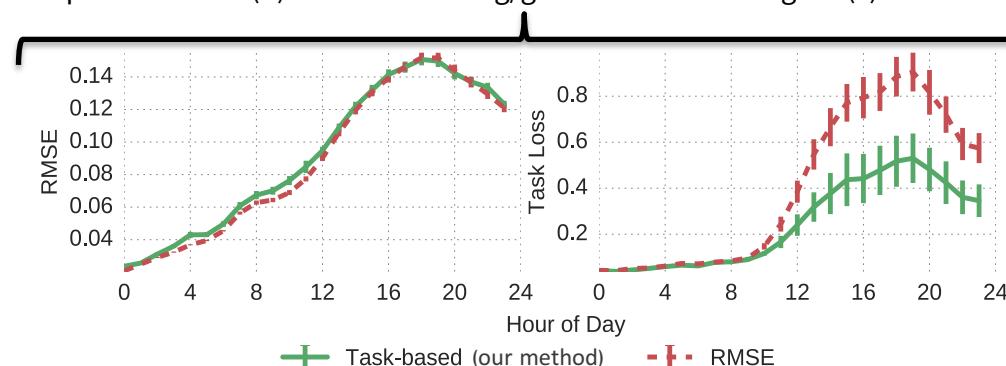
Idea: use the **downstream optimizer as a loss** for the model using differentiable optimization



(a) Inventory stock problem

(b) Load forecasting/generator scheduling

(c) Price forecasting/battery arbitrage



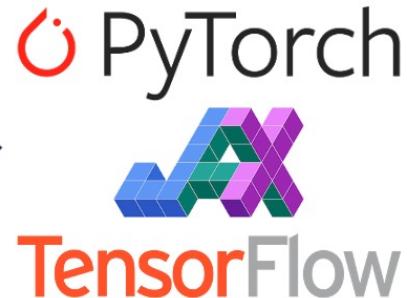
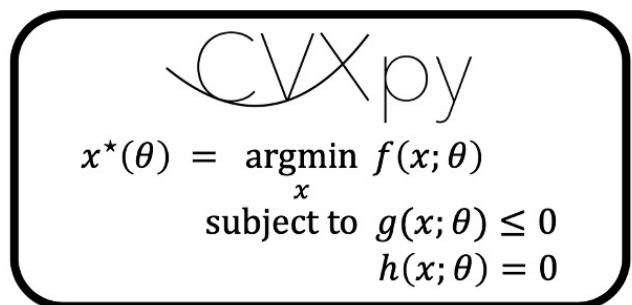
$$\underset{z \in \mathbb{R}^{24}}{\text{minimize}} \mathbf{E}_y \left[\sum_{i=1}^{24} \gamma_s [y_i - z_i]_+ + \gamma_e [z_i - y_i]_+ + \frac{1}{2} \|z_i - y_i\|^2 \right] \quad \text{subject to } |z_i - z_{i+1}| \leq c_{\text{ramp}}.$$

Implementing differentiable optimization

Manually: unroll or implicitly differentiate the optimality conditions (such as the KKT system)
My original differentiable QP implementation was **~1k lines of code** to make efficient

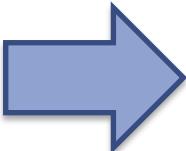
Use a software package to prototype such as:

- **cvxpylayers**: differentiable convex optimization in CVXPY [Agrawal*, Amos*, et al., NeurIPS 2019]
Implements a differentiable QP in ~10 lines of code
- **Theseus**: differentiable non-linear least squares with a focus on robotics [Pineda et al., NeurIPS 2022]
- **higher**: differentiable unrolled optimizers [Grefenstette et al., 2019]



Code example: OptNet QP

Before: 1k lines of code



Now: ~10 lines of code

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

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

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

```
1 Q = cp.Parameter((n, n), PSD=True)
2 p = cp.Parameter(n)
3 A = cp.Parameter((m, n))
4 b = cp.Parameter(m)
5 G = cp.Parameter((p, n))
6 h = cp.Parameter(p)
7 x = cp.Variable(n)
8 obj = cp.Minimize(0.5*cp.quad_form(x, Q) + p.T * x)
9 cons = [A*x == b, G*x <= h]
10 prob = cp.Problem(obj, cons)
11 layer = CvxpyLayer(prob, params=[Q, p, A, b, G, h], out=[x])
```

This talk

Differentiable optimization — $\frac{\partial}{\partial x} y^*(x)$

Foundations

Differentiable convex optimization layers

Differentiable control

Optimization-based task losses

Amortized optimization — $\hat{y}_\theta(x) \approx y^*(x)$

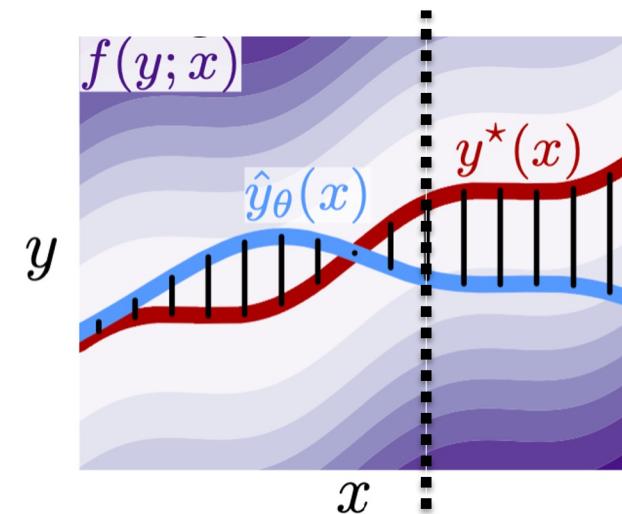
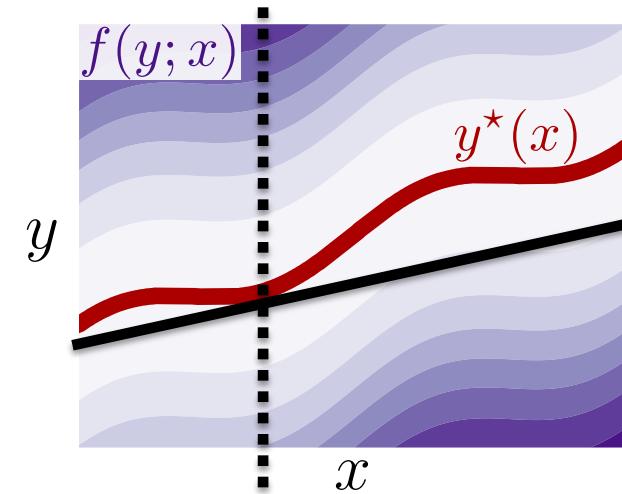
Foundations

RL as amortized optimization

Amortization via learning latent subspaces

Meta Optimal Transport

Amortizing convex conjugates



Difficulty: optimization is computationally expensive

Sometimes solving just **once** may be difficult

Exasperated when **repeatedly solving** during deployment

Insight: optimal solutions share structure

Optimization problems **share structure** and don't live in isolation

Solution: amortized optimization

Use **machine learning** to uncover the shared structure

Create **learning-augmented** versions of classical optimization solvers

Far surpasses average or worst-case convergence rates

Also referred to as **learning to optimize**

Amortized optimization

Two key components:

1. **Amortization model** $\hat{y}_\theta(x)$ tries to approximate $y^*(x)$

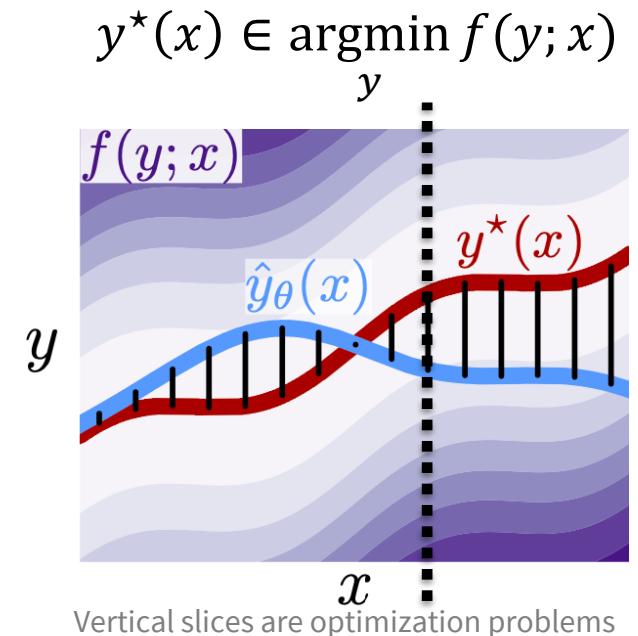
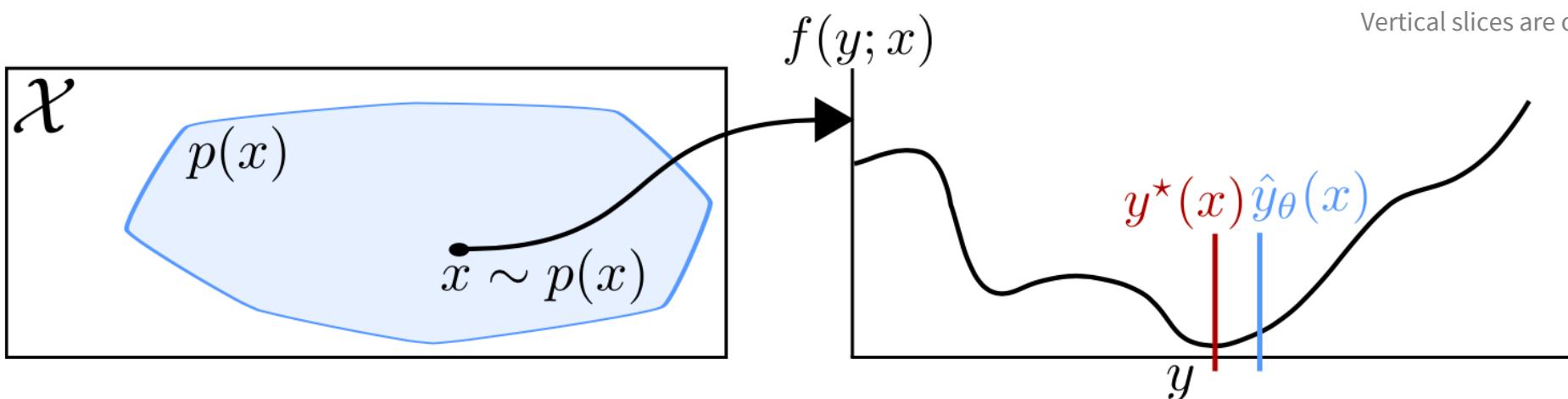
Fully-amortized: A neural network mapping from x to the solution

Semi-amortized: Allowed to query the objective f

2. **Loss** \mathcal{L} measures how well \hat{y} fits y^* and optimized with $\min_\theta \mathcal{L}(\hat{y}_\theta)$

Regression: $\mathcal{L}_{\text{reg}}(\hat{y}_\theta) := \mathbb{E}_{p(x)} \|\hat{y}_\theta(x) - y^*(x)\|_2^2$

Objective-based: $\mathcal{L}_{\text{obj}}(\hat{y}_\theta) := \mathbb{E}_{p(x)} f(\hat{y}_\theta(x); x)$



RL policy learning is amortized optimization

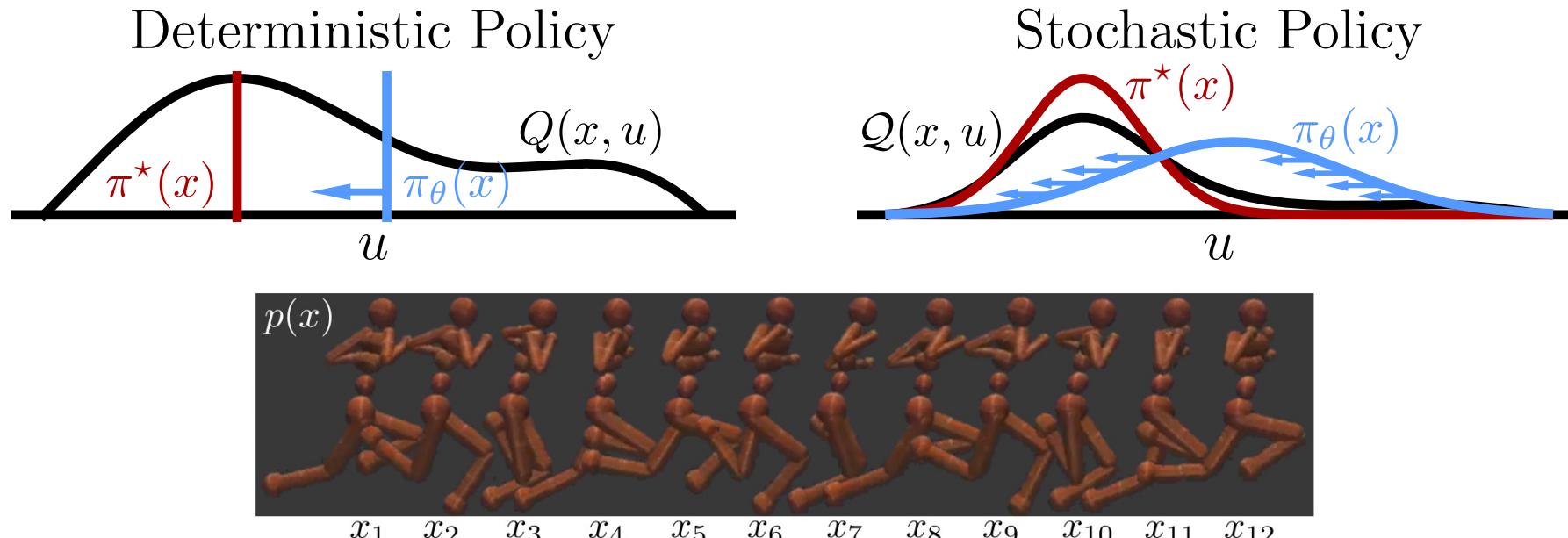
Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning (to appear)
On the model-based stochastic value gradient for continuous reinforcement learning. Amos et al., L4DC 2021.

Setup: controlling a **continuous MDP** with a **model-free policy** $\pi_\theta(x)$

Review: Learning a policy with a **value gradient** amortizes over the Q -value:

$$\operatorname{argmax}_\theta \mathbb{E}_{p(x)} Q(x, \pi_\theta(x))$$

The **amortization perspective** easily enables **expanding beyond this fully-amortized setting**



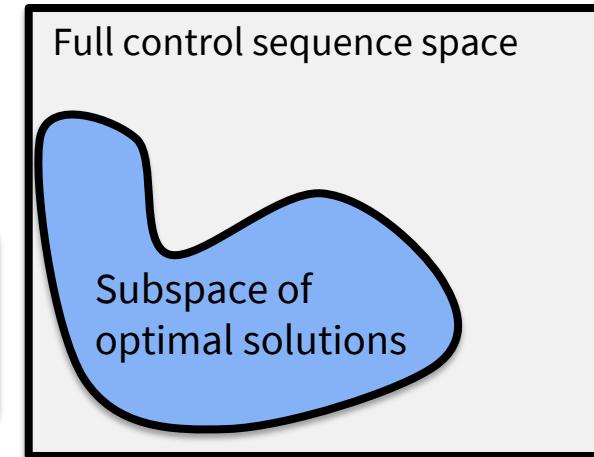
Amortization via learning latent subspaces

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

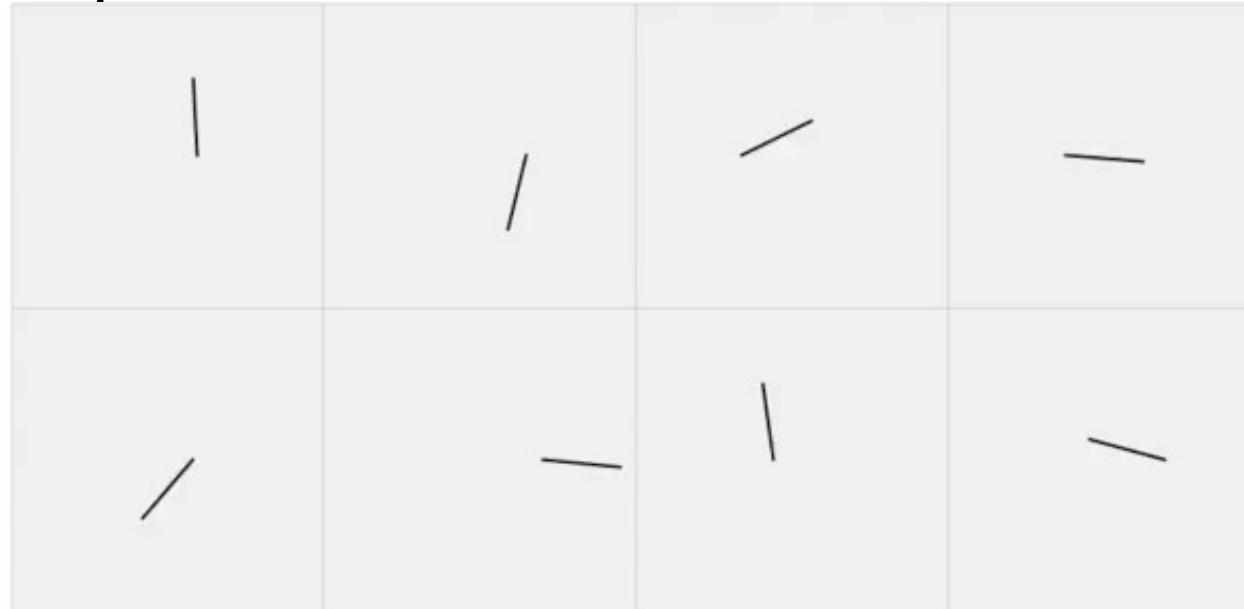
Amortize the problem by learning a latent subspace of optimal solutions

Only search over optimal solutions rather than the entire space

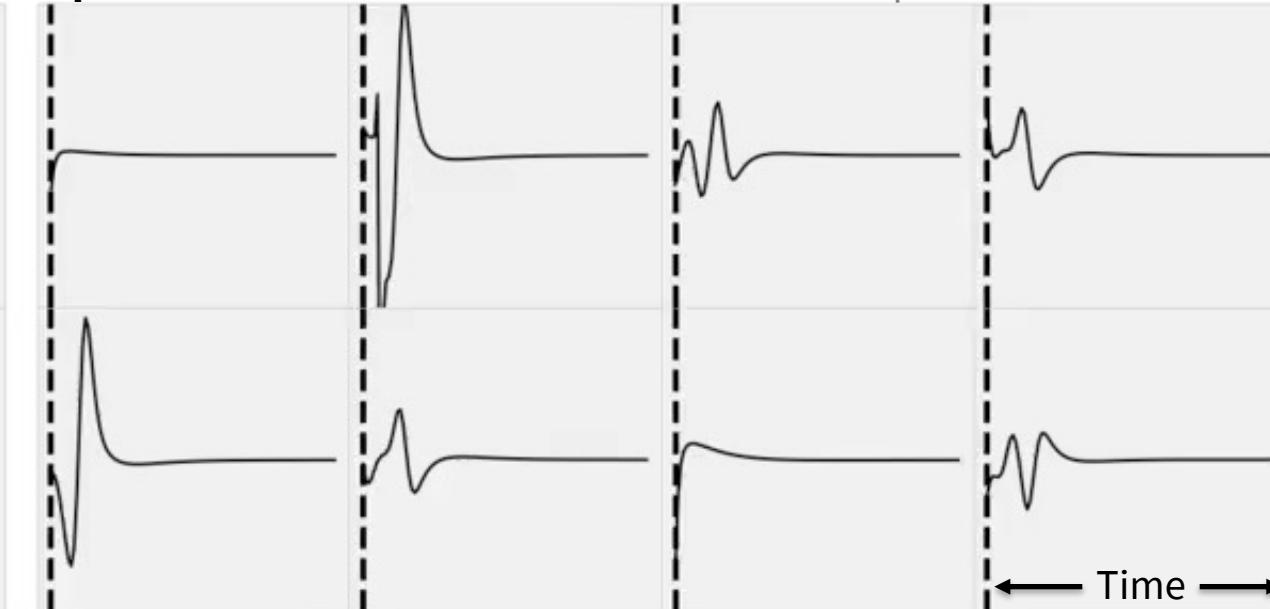
$$x_{1:T}^*, u_{1:T}^* \in \operatorname{argmin}_{x_{1:T}, u_{1:T}} \sum_t \text{cost } C_\theta(x_t, u_t) \text{ s.t. } \begin{array}{l} \text{initial state } x_1 = x_{\text{init}} \\ \text{dynamics } x_{t+1} = f_\theta(x_t, u_t) \\ \text{constraints } u_t \in \mathcal{U} \end{array}$$



Cartpole videos



Optimal controls over time — force on the cartpole



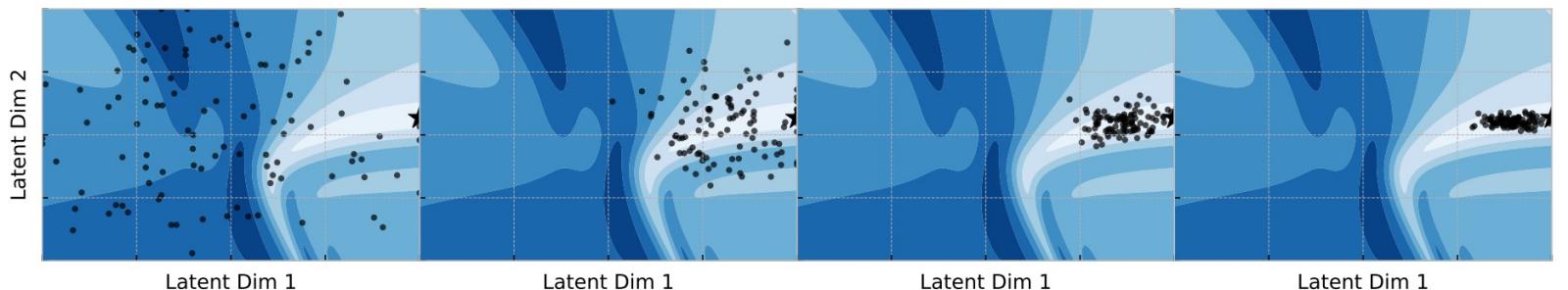
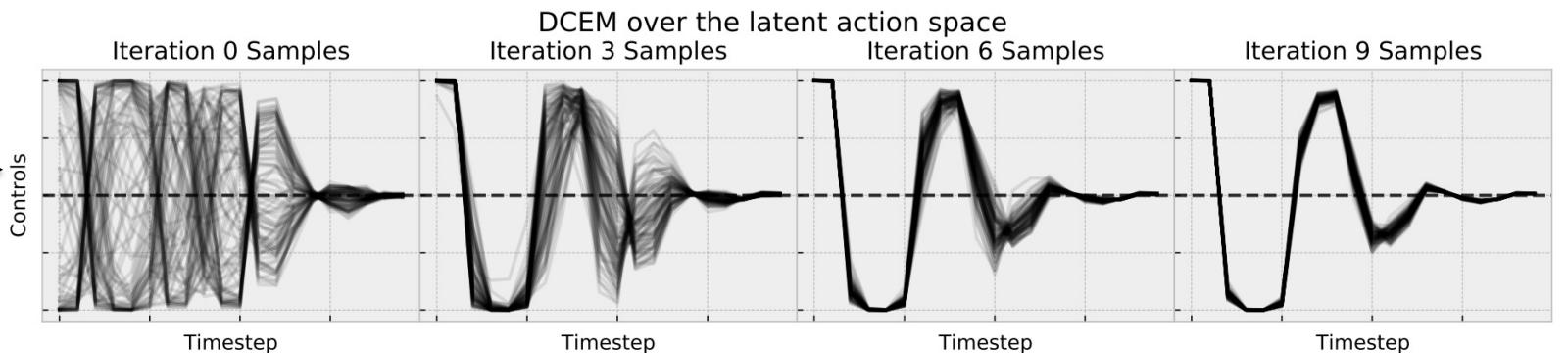
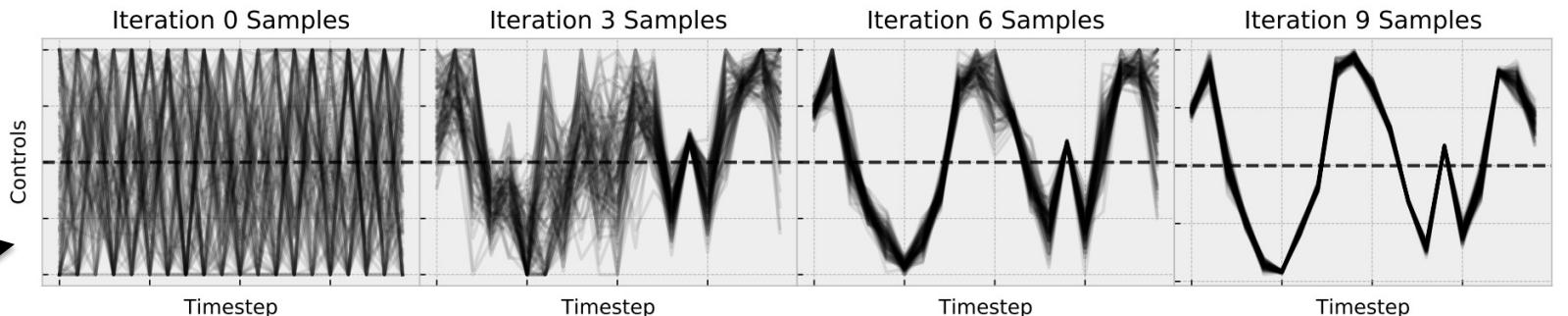
Amortization via learning latent subspaces

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

CEM over the full action space

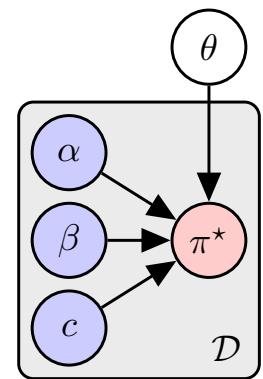
$$u^* = \operatorname{argmin}_{u \in [0,1]^N} f(u)$$

Full control sequence space



Meta Optimal Transport

[Amos et al., 2022]

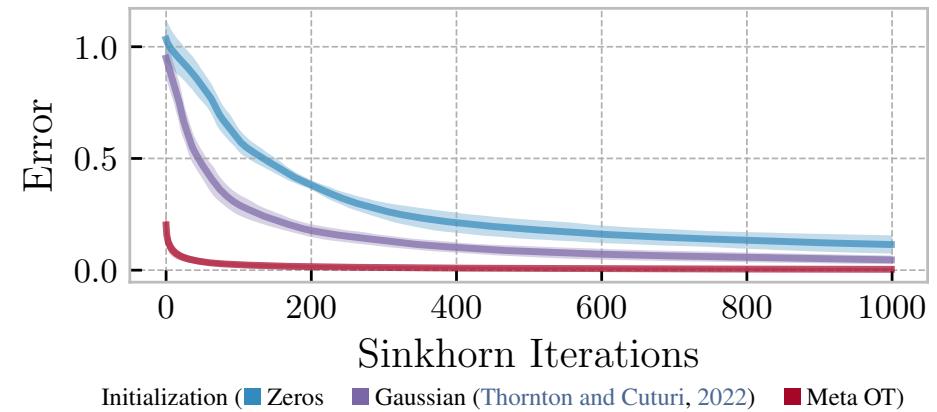


Goal: optimally transport mass between measures α to β

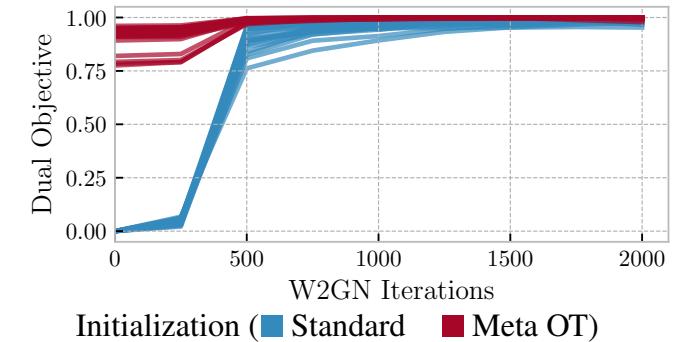
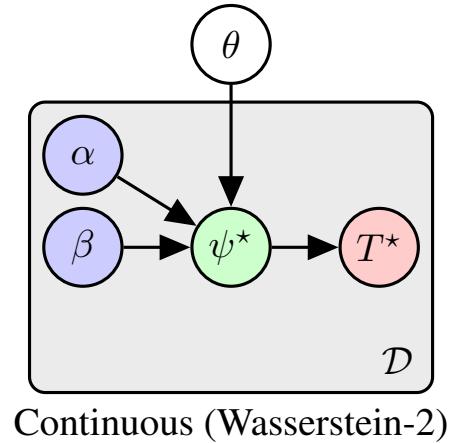
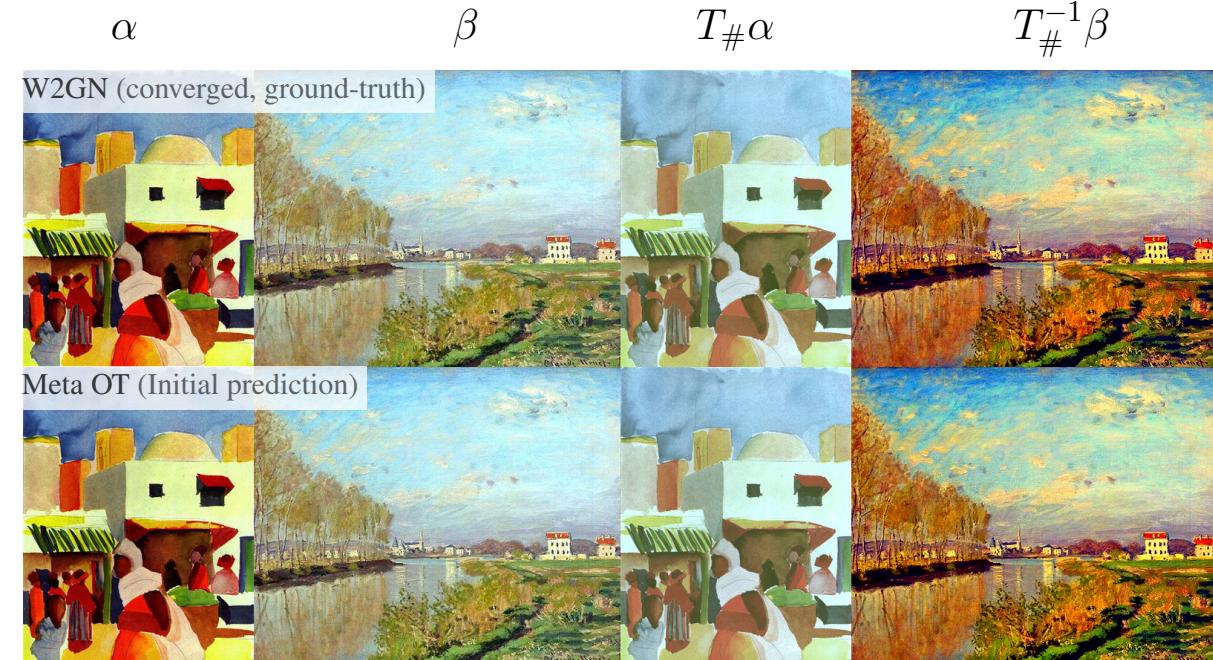
$$\pi^*(\alpha, \beta, c) \in \operatorname{argmin}_{\pi \in \mathcal{U}(\alpha, \beta)} \int_{X \times Y} c(x, y) d\pi(x, y)$$

Use **amortization** when **repeatedly coupling measures**
e.g., between pairs of images or physical transport

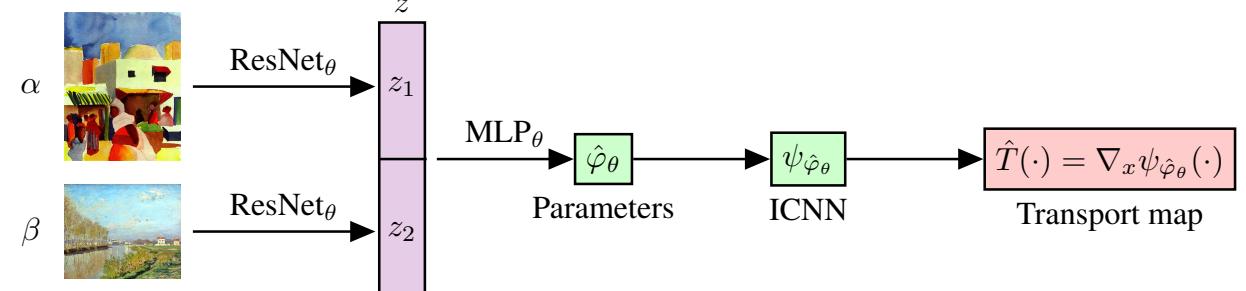
Often amortize over **unconstrained dual potentials**



Meta OT for continuous OT with Meta ICNNs



Meta ICNN: Predict parameters of ICNN coupling α and β



More Meta OT color transfer predictions

α

β

$T_{\#}\alpha$

$T_{\#}^{-1}\beta$

α

β

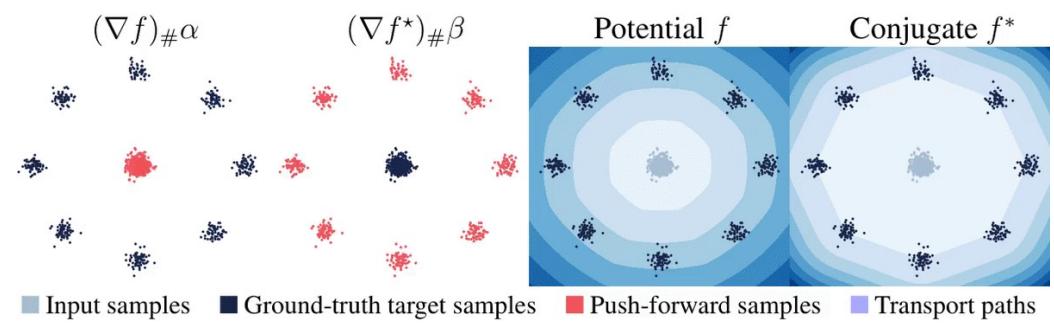
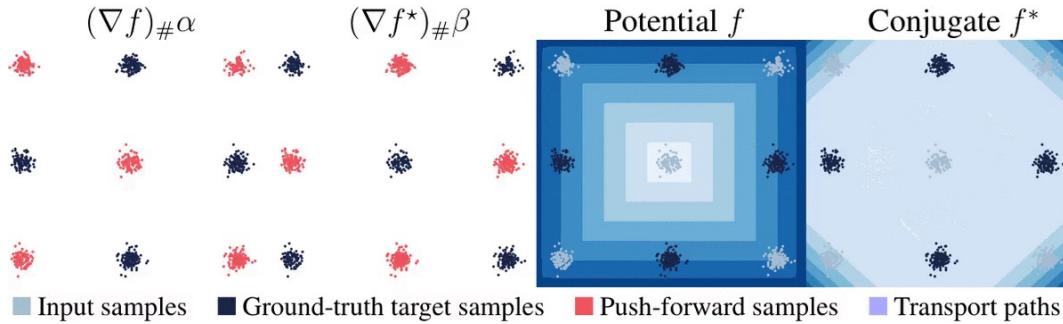
$T_{\#}\alpha$

$T_{\#}^{-1}\beta$



On amortizing convex conjugates for OT

[Amos, 2022]



Setting: transport between measures α and β

Monge problem for Euclidean Wasserstein-2

$$T^*(\alpha, \beta) \in \operatorname{argmin}_{T \in \mathcal{C}(\alpha, \beta)} \mathbb{E}_{x \sim \alpha} \|x - T(x)\|_2^2$$

$$T^* = \nabla \hat{f} \text{ from Brenier's theorem}$$

$f^*(y) := -\inf_x f(x) - x^\top y$ is the convex conjugate

Kantorovich dual

$$\hat{f} \in \operatorname{argmax}_{f \in \mathcal{L}^1(\alpha)} -\mathbb{E}_{x \sim \alpha}[f(x)] - \mathbb{E}_{y \sim \beta}[f^*(y)]$$

Challenge: The **convex conjugate can be computationally expensive** to numerically estimate

Idea: Amortize and fine-tune the conjugate to rapidly estimate it

Improves Wasserstein-2 benchmark results by **~2-4x**

Closing thoughts

Optimization expresses **non-trivial reasoning operations**

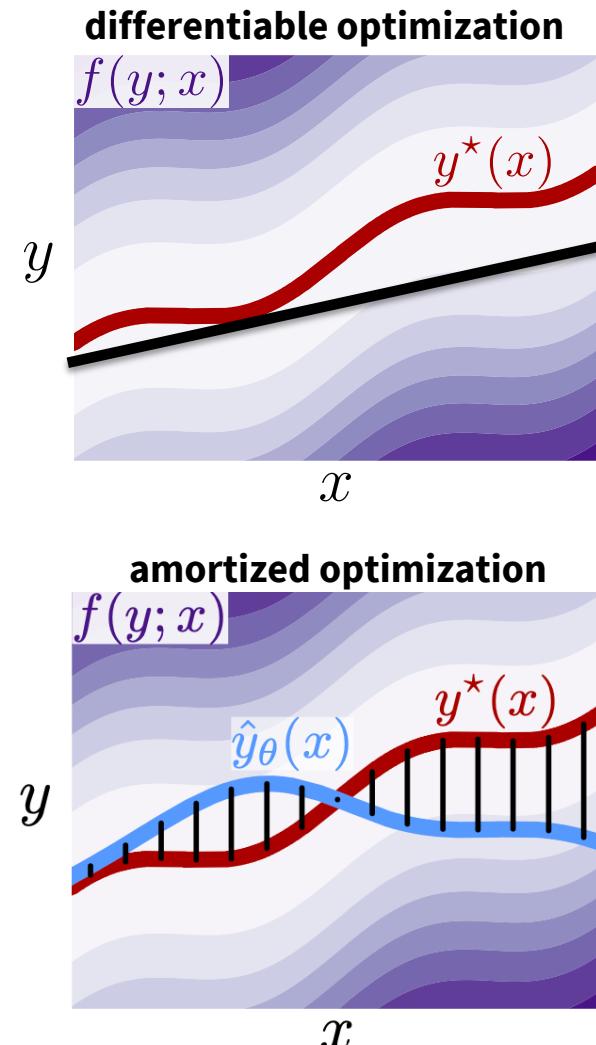
- Integrates nicely with machine learning systems by **seeing it as a function**

Differentiable optimization is a powerful primitive within larger systems

- Theoretical and engineering foundations are here
- Can be propagated through and learned, just like any layer
- Provides a perspective to analyze existing models and layers

Amortized optimization enables fast learning-augmented solvers

- Foundations are likewise here
- Provides a perspective on existing methods in RL, VI, OT



Future directions

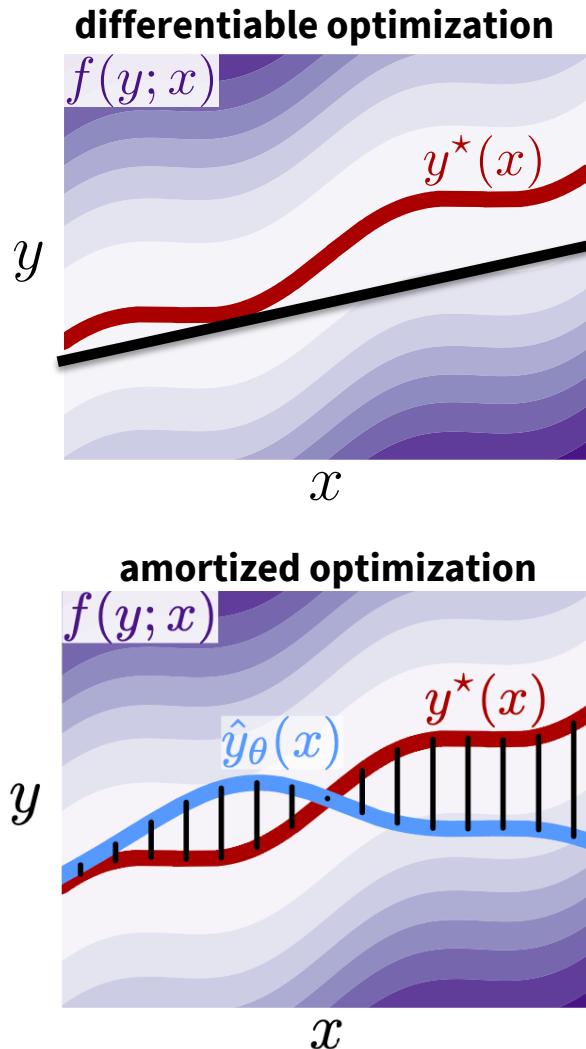
Goal: build intelligent systems that understand and interact with the world
Advancing **optimization** and **machine learning foundations** is crucial

Differentiable optimization — $\frac{\partial}{\partial x} y^*(x)$

- *Differentiable control: learning control-aware representations*
- *Numerics: “differentiating” ill-behaved functions*
- *Generalizing to non-convex or non-Euclidean settings*

Amortized optimization — $\hat{y}_\theta(x) \approx y^*(x)$

- *Numerics: amortizing with distributions and Markov kernels*
- *Building general learning-augmented optimizers*
- *Amortization models that use differentiable optimization*

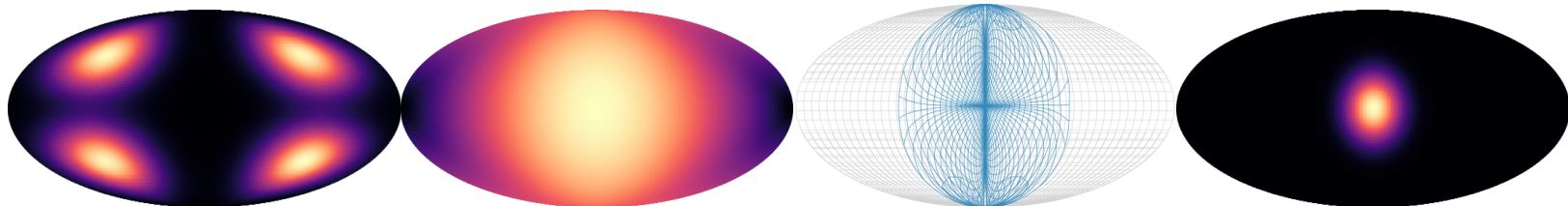


Learning foundations beyond optimization

I want to **build intelligent systems** that **understand and interact with the world**
Advancing **optimization** and **machine learning foundations** is crucial

Next frontier includes understanding, mapping between, and optimizing over:

- **Modeling and controlling non-trivial physical systems** (e.g. fluid dynamics, open-world robots)
- **High-dimensional** image, video, and text spaces
- **Discrete structures** arising from decisions (e.g. the knapsack) and other natural structures
- **Riemannian geometries** expressing 3D objects and many other mathematical spaces
- **Optimal transport** connecting spaces and geometries



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

Learning with differentiable and amortized optimization

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[ICML 2017] [Differentiable QPs: OptNet](#)

[NeurIPS 2017] [Differentiable Task-based Model Learning](#)

[NeurIPS 2018] [Differentiable MPC for End-to-end Planning and Control](#)

[NeurIPS 2019] [Differentiable Convex Optimization Layers](#)

[Ph.D. Thesis 2019] [Differentiable Optimization-Based Modeling for ML](#)

[arXiv 2019] [Differentiable Top-k and Multi-Label Projection](#)

[arXiv 2019] [Generalized Inner Loop Meta-Learning](#)

[ICML 2020] [Differentiable Cross-Entropy Method](#)

[ICML 2021] [Differentiable Combinatorial Optimization: CombOptNet](#)

[L4DC 2021] [On the model-based stochastic value gradient](#)

[NeurIPS 2022] [Theseus: Differentiable Nonlinear Optimization](#)

[arXiv 2022] [Meta Optimal Transport](#)

[arXiv 2022] [On amortizing convex conjugates for optimal transport](#)

[Foundations and Trends in ML, to appear] [Tutorial on amortized optimization](#)

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