Tutorial on amortized optimization for learning to optimize over continuous spaces

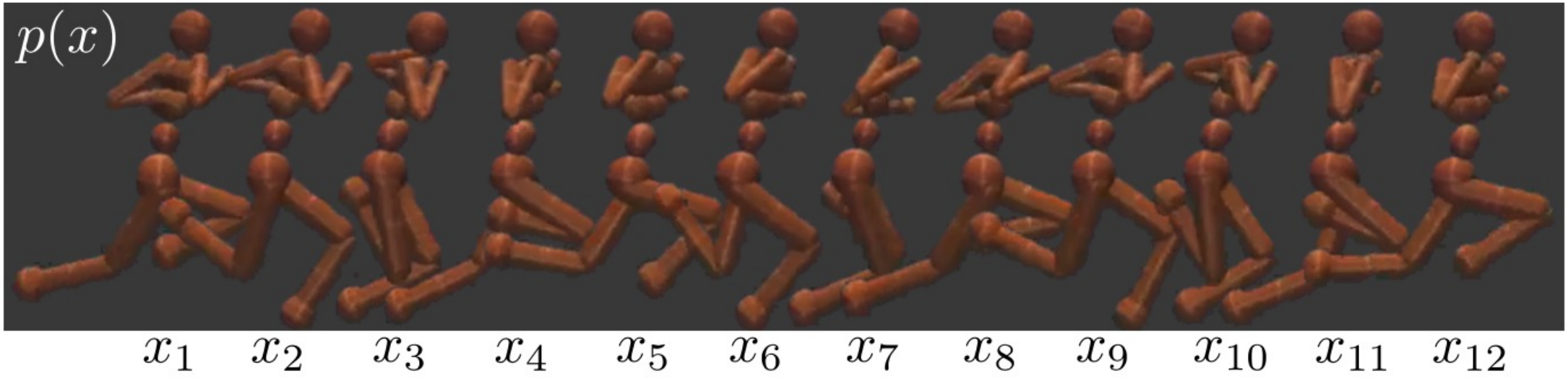
Brandon Amos, Meta AI (FAIR) brandondamos bamos.github.io

Optimization is a powerful modeling tool

Continuous optimization expresses many **non-trivial operations**

Control, reinforcement learning, robotics, geometry (projections), variational inference, finance (portfolio optimization), sparse coding, meta-learning, deep equilibrium networks, optimal transport, game and market equilibrium

Application: Continuous control of a robotic system:



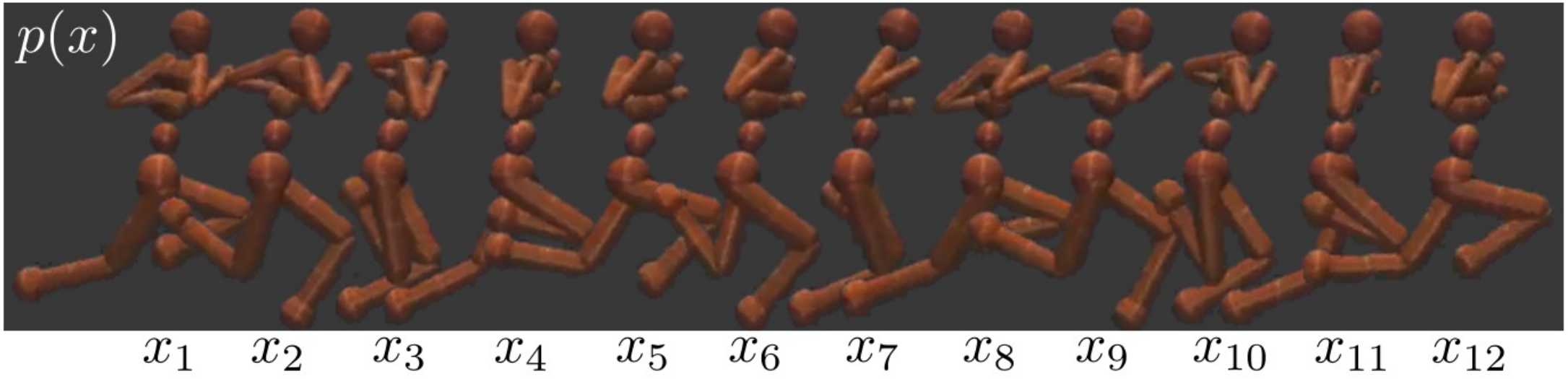
Repeatedly solving optimization problems

Optimization problems often **do not live in isolation** and are often **repeatedly solved** in deployment

$$y^\star(x) \in \operatorname{argmin}_y f(y; x)$$

Optimal solution | Optimization variable | Objective | Context

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



Difficulty: Optimization is computationally expensive

Sometimes solving just **once** may be difficult
Exasperated when **repeatedly solving** during deployment

Insight: Shared structure between problems

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

Amortized optimization foundations

This talk: Explore foundations and connect applications

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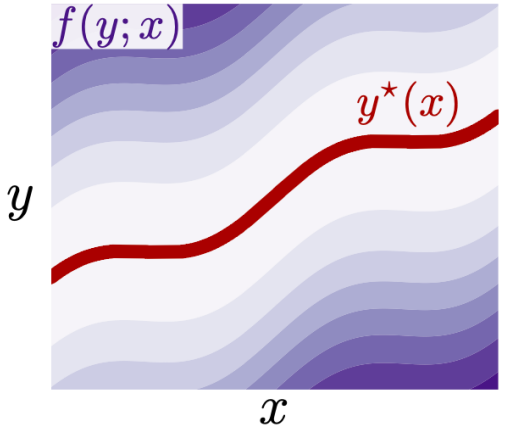
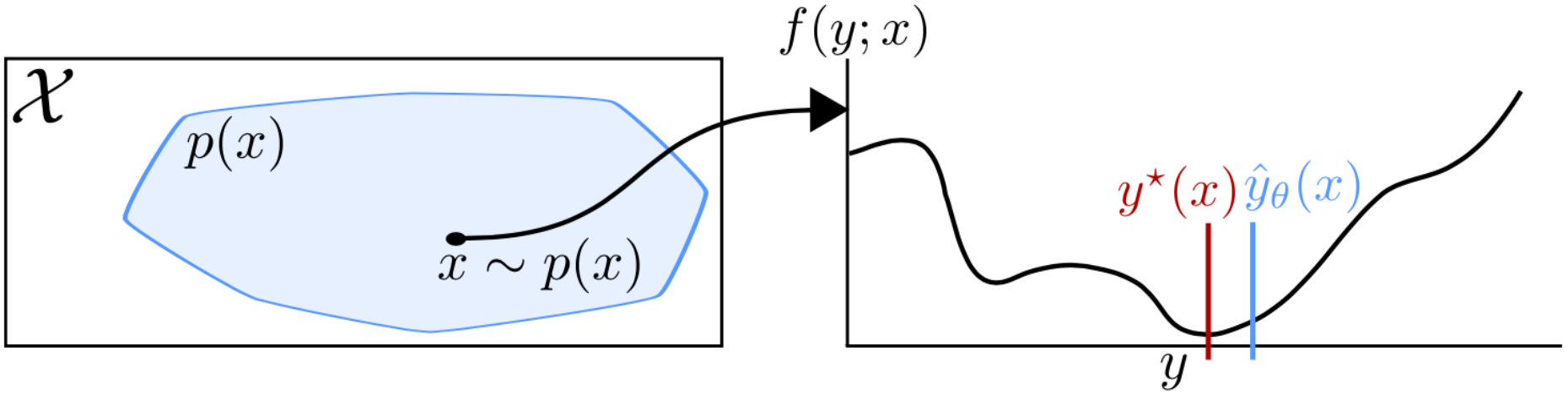


Amortization model $\hat{y}_\theta(x)$ tries to approximate $y^\star(x)$

Example: A neural network mapping from x to the solution

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

Example: $\mathcal{L}(\hat{y}_\theta) \coloneqq \mathbb{E}_{p(x)} \|\hat{y}_\theta(x) - y^\star(x)\|_2^2$



This talk: Amortized optimization

Motivation and context

Design decisions
- Modeling paradigms for $\hat{y}_\theta$ (fully-amortized and semi-amortized models)
- Learning paradigms for $\mathcal{L}$ (objective-based and regression-based)

Applications
- VAEs, hyper-networks, MAML, reinforcement learning, meta optimal transport

Extensions and limitations

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Modeling paradigms for $\hat{y}_\theta$

Fully-amortized models: Map from the context x to the solution **without** accessing the objective f
Example: Neural network mapping from x to the solution
Most of our applications will focus on these

Semi-amortized models: Internally access the objective f
Example: Gradient-based meta-learning models such as MAML

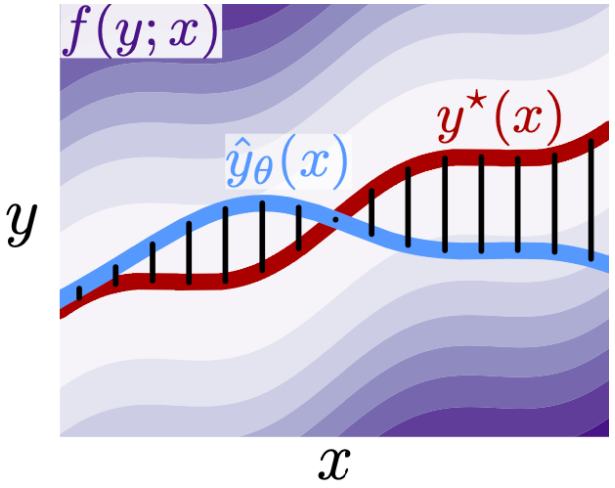
$$\hat{y}_\theta^0 \rightarrow \hat{y}_\theta^1 \rightarrow \cdots \rightarrow \hat{y}_\theta^K =: \hat{y}_\theta(x)$$

Learning paradigms for $\mathcal{L}$

Regression-based

$$\mathcal{L}_{\text{reg}}(\hat{y}_\theta) \coloneqq \mathbb{E}_{p(x)} \|\hat{y}_\theta(x) - y^\star(x)\|_2^2$$

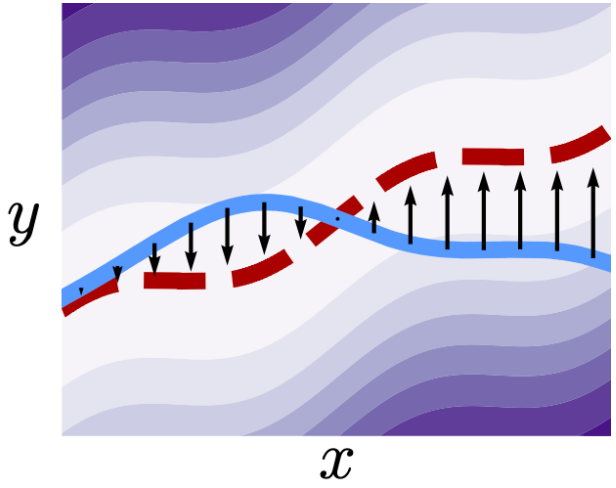
- $-$ Does not consider $f(y; x)$
- $+$ Uses global information with $y^\star(x)$
- $-$ Expensive to compute $y^\star(x)$
- $+$ Does not compute $\nabla_y f(y; x)$
- $-$ Hard to learn non-unique $y^\star(x)$



Objective-based:

$$\mathcal{L}_{\text{obj}}(\hat{y}_\theta) \coloneqq \mathbb{E}_{p(x)} f(\hat{y}_\theta(x); x)$$

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



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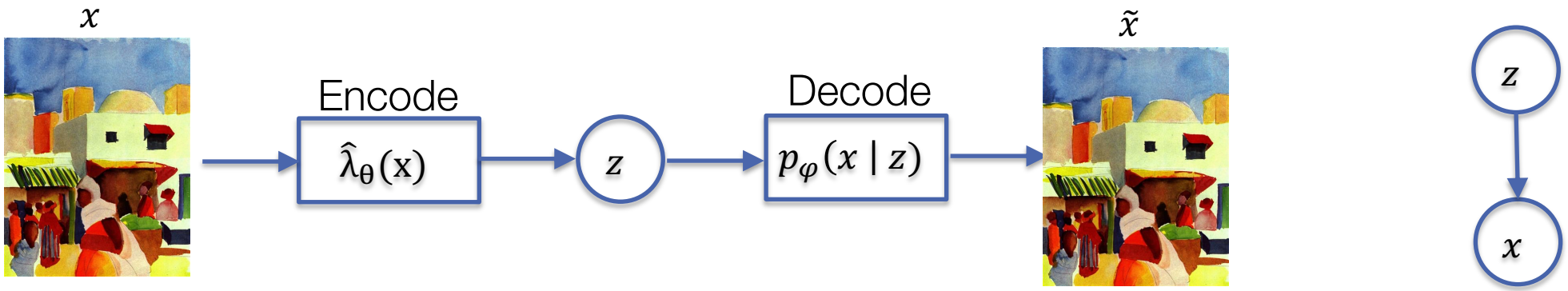
Warning: Quick overview of separate applications

Goal: Give a broad overview of **existing uses of amortized optimization**
Will try to focus on the amortization components, but assumes some context

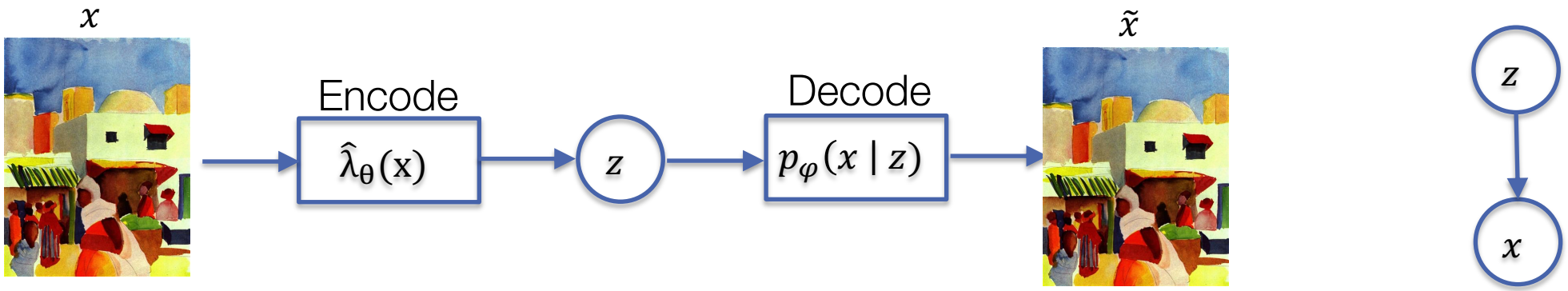
Amortized variational inference and auto-encoders



VAEs amortize the evidence lower bound (ELBO)

model: fully-amortized $\hat{\lambda}_\theta(x)$ as a neural network
loss: objective-based
objective: ELBO
learning: $\max_{\theta,\varphi} \mathbb{E}_{p(x)} \, \text{ELBO}(\hat{\lambda}_\theta(x); x, \varphi)$

Semi-amortized variational autoencoders



Incorporates knowledge of the ELBO into the encoder

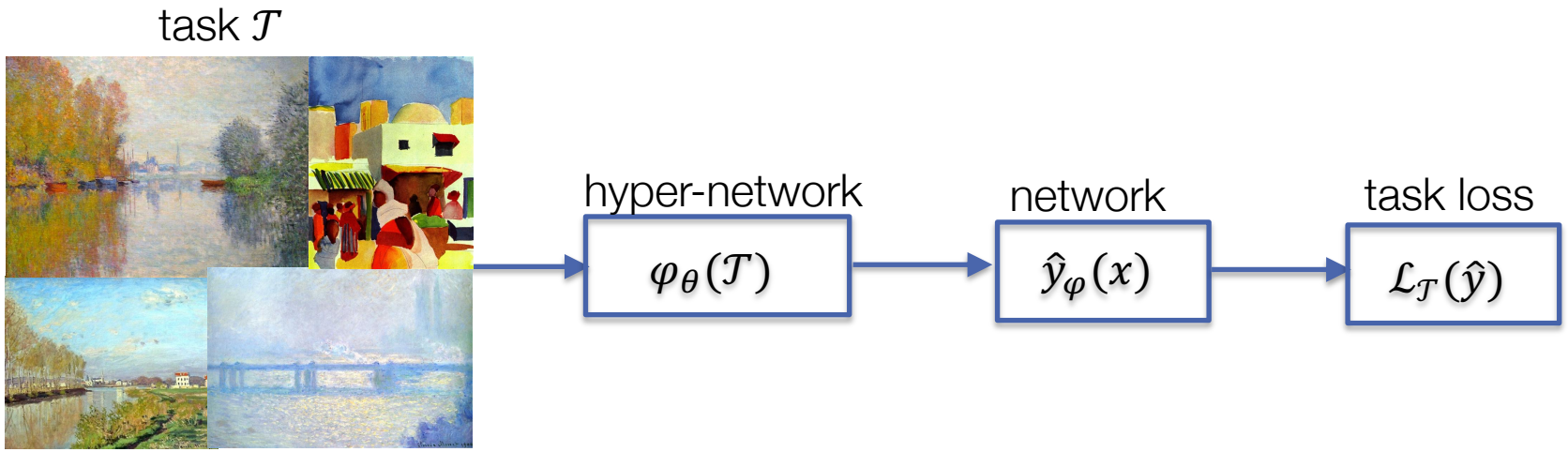
model: semi-amortized $\hat{\lambda}_\theta(x) \approx \underset{\lambda}{\operatorname{argmin}}\, \mathrm{ELBO}(\lambda; x, \varphi)$, approximated by gradient updates

loss: objective-based

objective: ELBO (same as before)

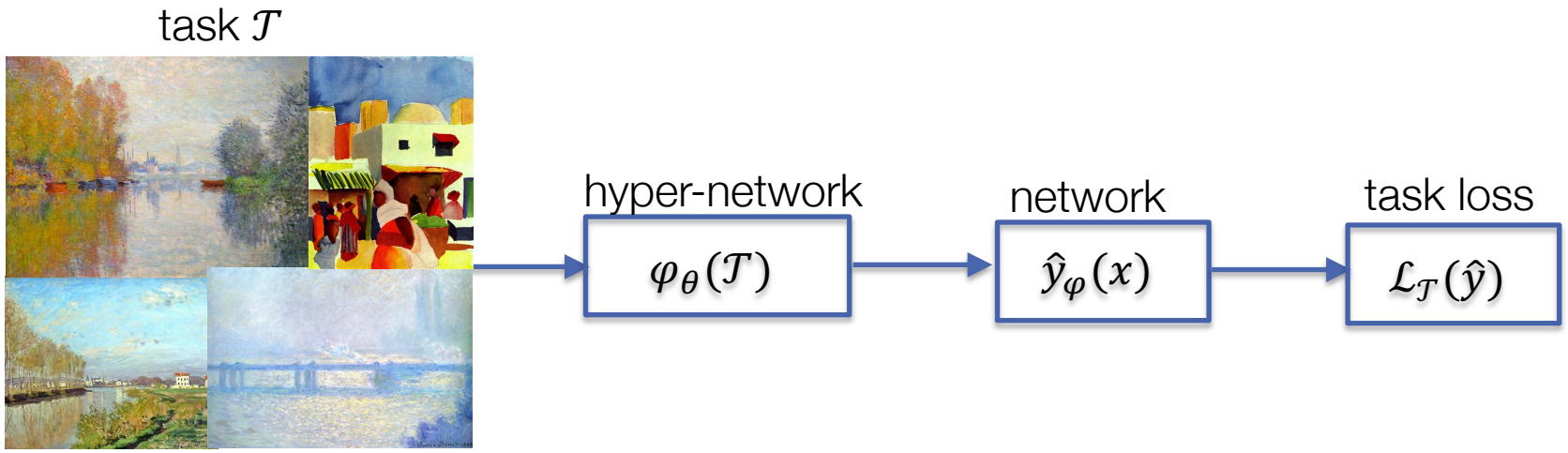
learning: $\max_{\theta,\varphi} \mathbb{E}_{p(x)}\, \mathrm{ELBO}(\hat{\lambda}_\theta(x); x, \varphi)$

Hyper-networks as amortized optimization



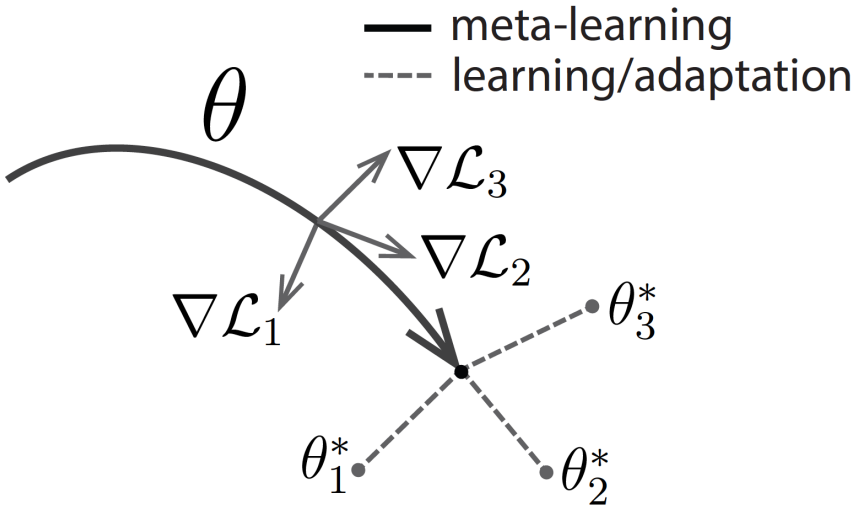
model: fully-amortized
loss: objective-based
objective: task loss
learning: $\underset{\theta}{\text{argmin}}\, \mathbb{E}_{p(\mathcal{T})}\, \mathcal{L}_\mathcal{T}(\hat{y})$

MAML as amortized optimization



Setup almost identical to hyper-networks, except for the model

model: semi-amortized
loss: objective-based
objective: task loss
learning: $\min_\theta \mathbb{E}_{p(\mathcal{T})} \mathcal{L}_\mathcal{T}(\hat{y}_\theta)$

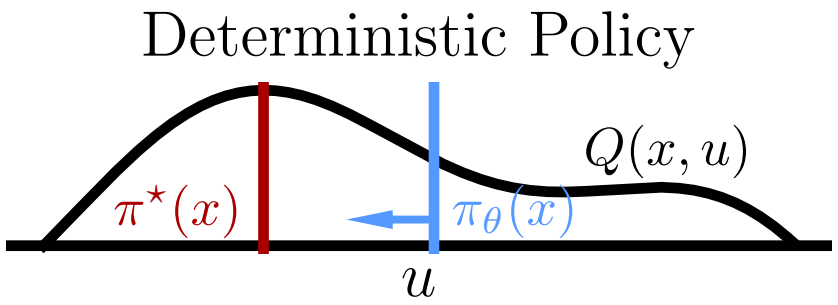


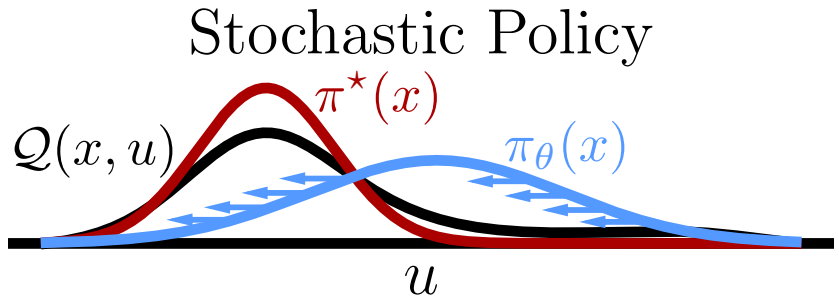
Amortized policy learning in reinforcement learning

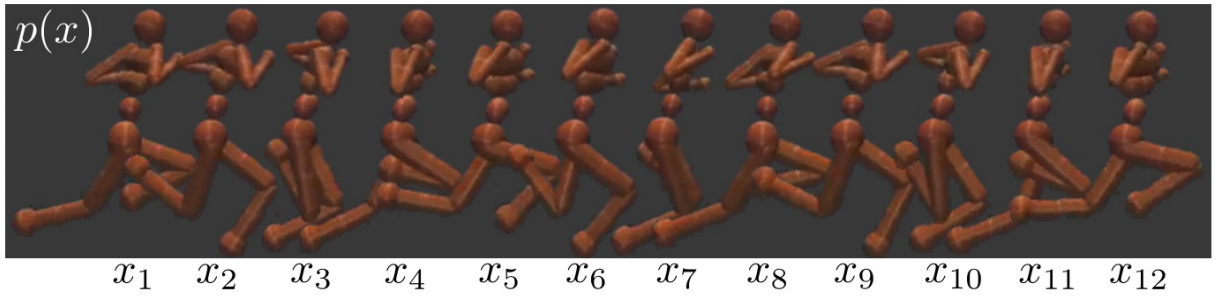
The **policy** $\pi_\theta(x)$ of almost every reinforcement learning method performs amortized optimization

setup: Controlling a continuous MDP
policy: $\pi_\theta(x)$
value (expected reward): $V(x) \coloneqq \mathbb{E}\, r(x_t, u_t)$
Q-value: $Q(x,u) \coloneqq \sum r(x,u) + \mathbb{E}_{x'} V^\pi(x')$

model: fully-amortized
loss: objective-based
objective: Q-value
learning: $\max_\theta \mathbb{E}_{p(x)}\, Q(x, \pi_\theta(x))$

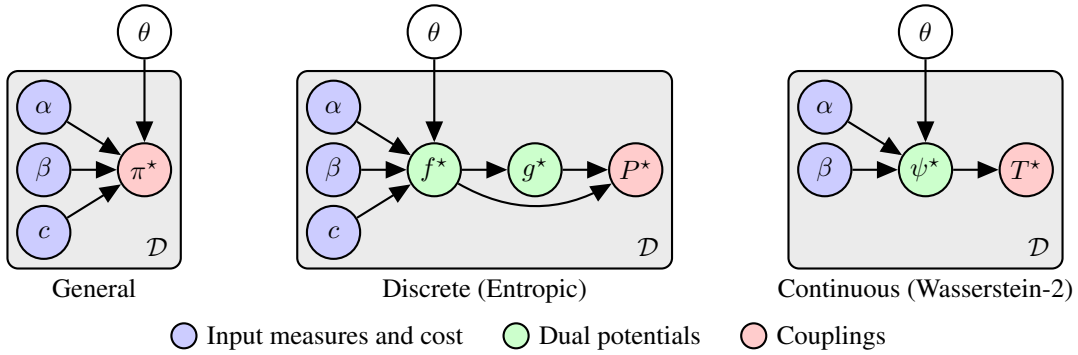


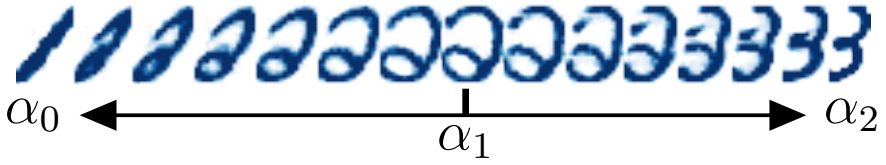


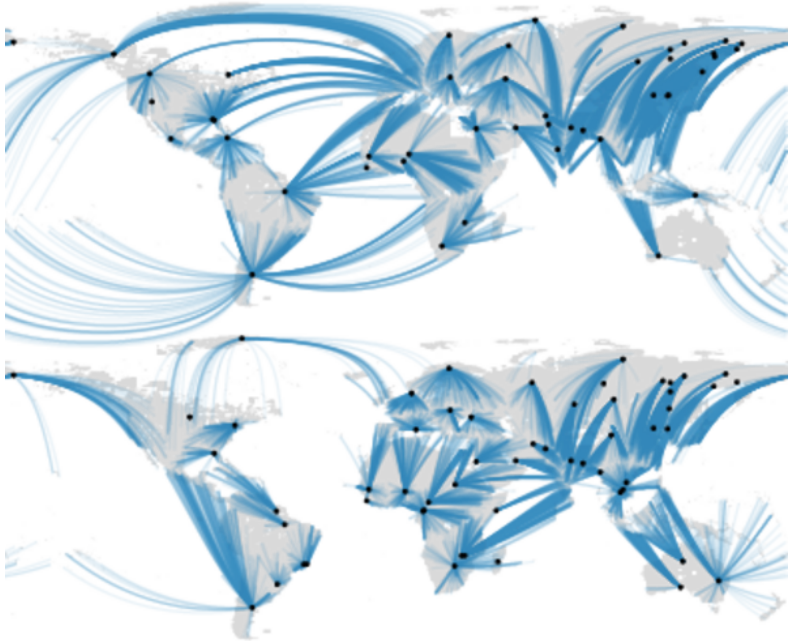


(Amortized) meta optimal transport

(Available on workplace)





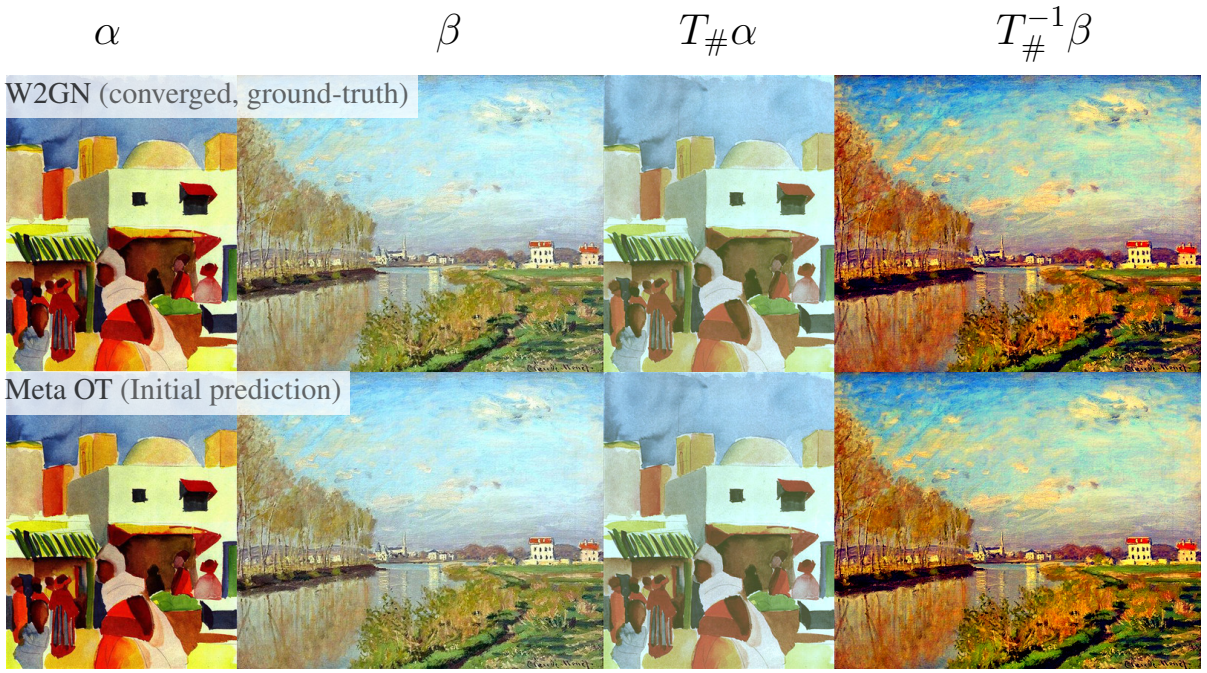


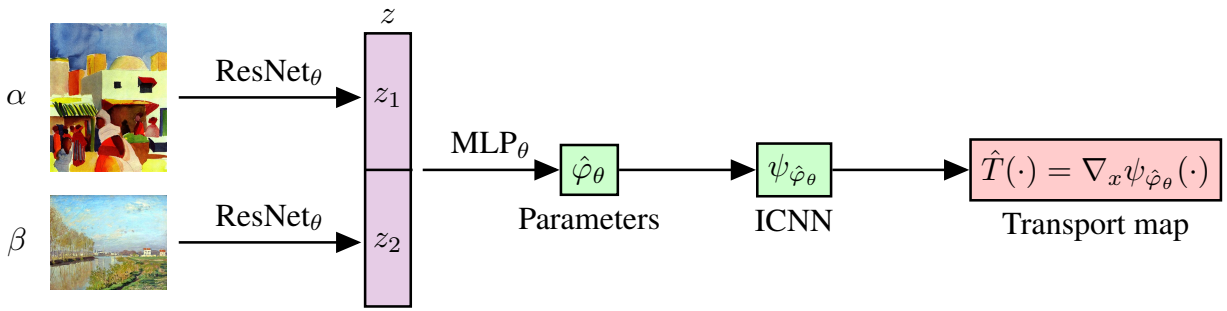
goal: Optimally transport mass between measures α to β

model: fully-amortized (hyper-network)
loss: objective-based
objective: transport cost
learning: $\max_{\theta} \mathbb{E}_{p(\alpha,\beta)} C(\hat{\pi}(\alpha,\beta))$

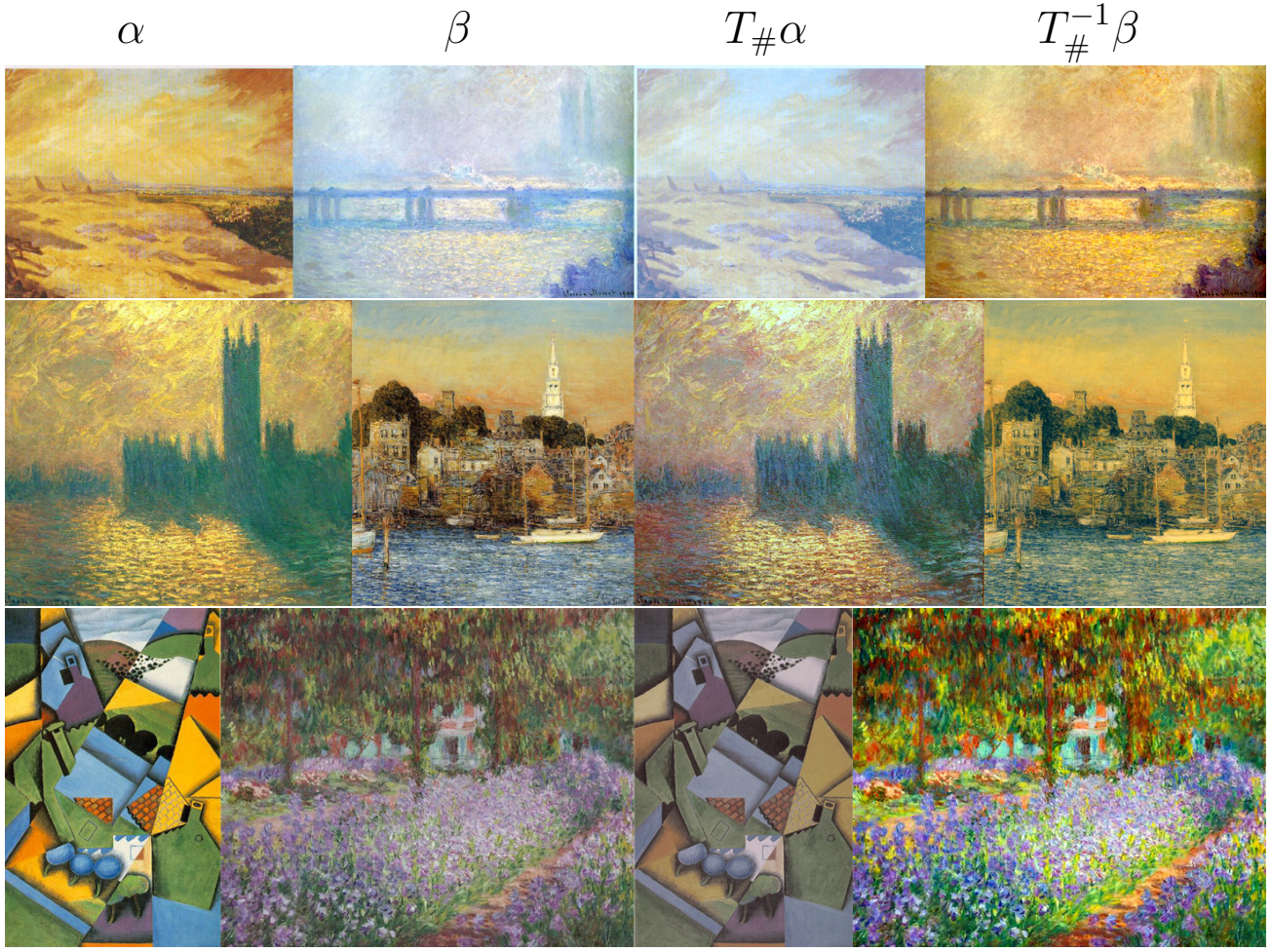
(Amortized) meta optimal transport

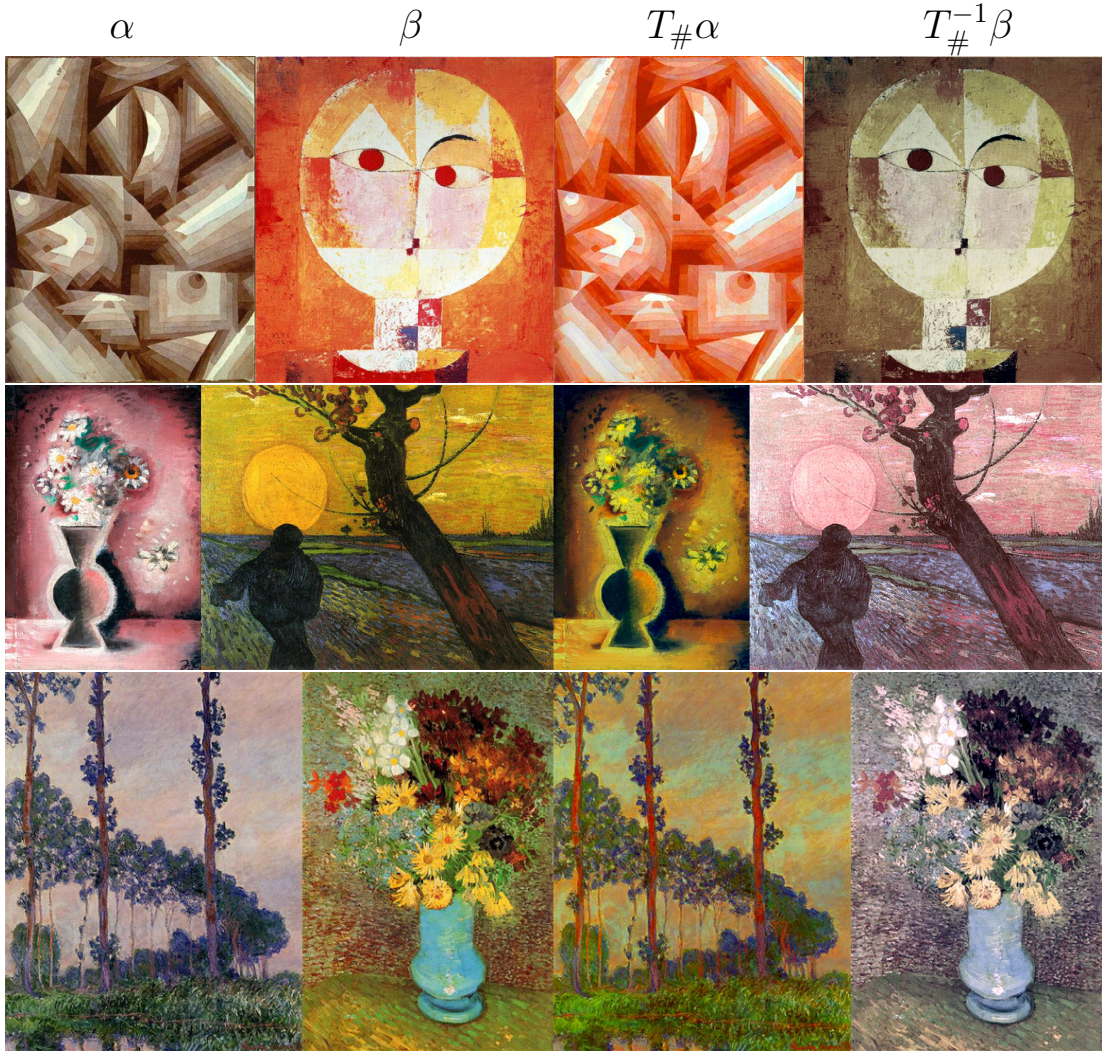
Predict couplings **10000x faster** than SOTA solvers that doesn't use learning





More meta color transfer predictions





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Extensions and limitations

Limitations of amortized optimization

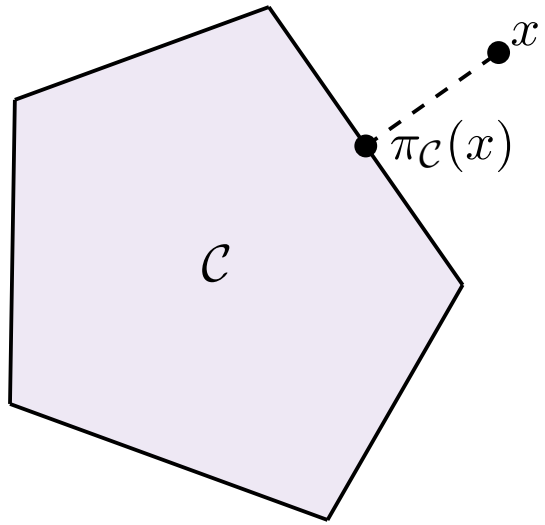
Gives extreme computational advantages in many settings
but may be detrimental and suboptimal in the wrong settings

1. Difficult in **out-of-domain settings** when the contexts significantly change
2. Generally difficult to **ensure stability or convergence**
3. Typically **does not solve previously intractable problems**
4. Can be **difficult to obtain high-accuracy solutions** without fine-tuning/semi-amortization

Extensions

All settings here: **unconstrained continuous Euclidean optimization problems**
Possible to expand far beyond these:

1. **New applications and settings for semi-amortized modeling**
2. **Constrained domains** (e.g. with differentiable projections)
3. **Discrete optimization settings** (e.g. with differentiable discrete optimization)
4. **Non-Euclidean settings** (e.g. with Riemannian optimization)



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github.com/facebookresearch/amortized-optimization-tutorial