Learning to Optimize

Ke Li
Jitendra Malik

Introduction

- Machine learning operates on a data-driven philosophy that favours automatic pattern discovery over manual design.
- Yet, the algorithms that power machine learning are still manually designed.
- Can we learn these algorithms instead?

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Learning to Learn

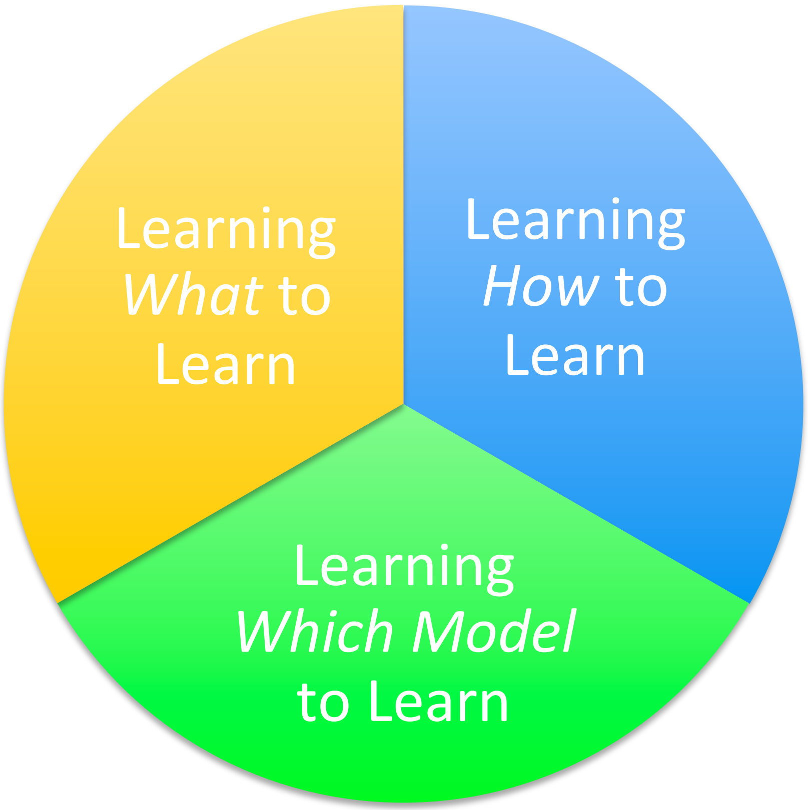
- Inspired by metacognition (Aristotle, 350 BC), which refers to the ability of humans to reason about their own process of reasoning.
- Goal: learn some general knowledge about the learning outcome or process that is useful across many tasks.
  - Unlike ordinary learning, generalization is not across instances, but across tasks.
- Terms:
  - Base-learning: instance-level learning
  - Meta-learning: task-level learning

Fundamental Challenge

- Key Problem: how do we parameterize the space of all possible learning methods such that it is both:
  1) expressive, and
  2) efficiently searchable?
- Two Extremes:
  – Enumerate a small set of methods: not expressive.
  – Search over all general-purpose programs: takes exponential time.

Learning to Learn

Different methods differ in the type of meta-knowledge they learn.



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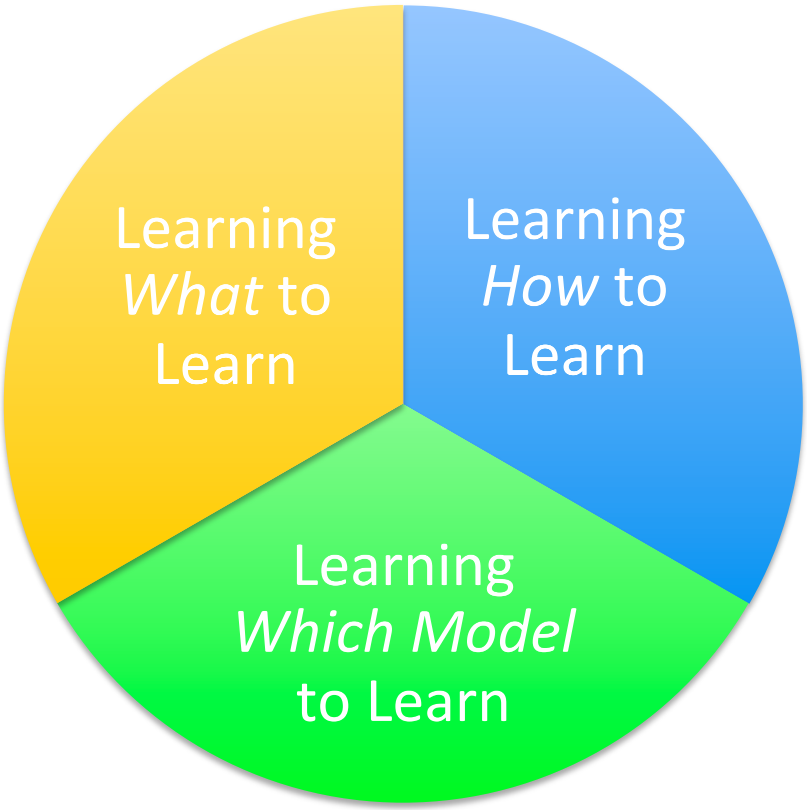
Learn parameter values of the base-model that are useful across tasks.



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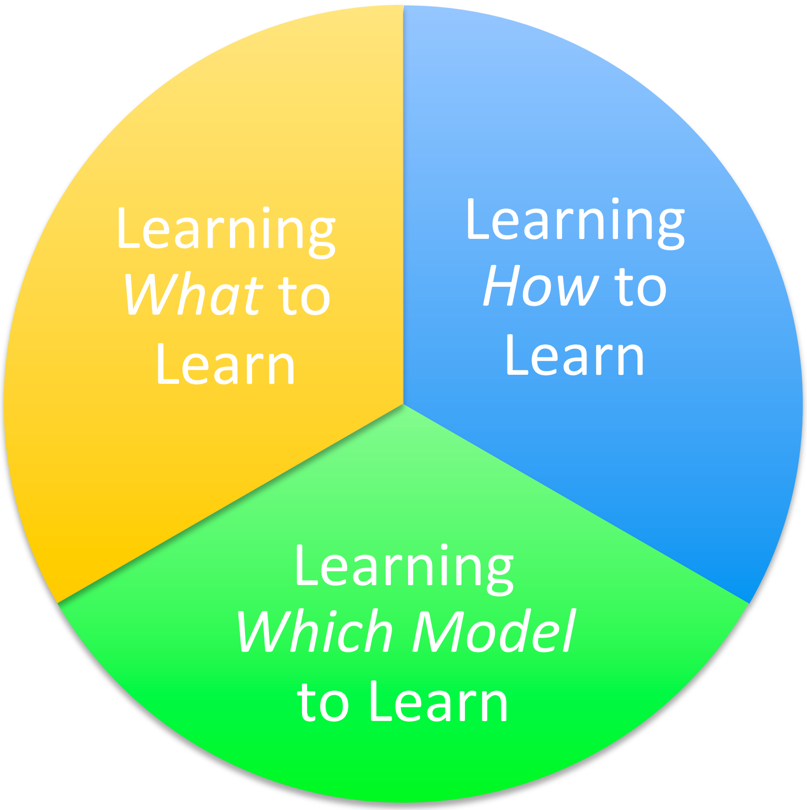
Learning to Learn

Different methods differ in the type of meta-knowledge they learn.

Learn parameter values of the base-model that are useful across tasks.

- Transfer Learning
- Multi-Task Learning
- Few-Shot Learning



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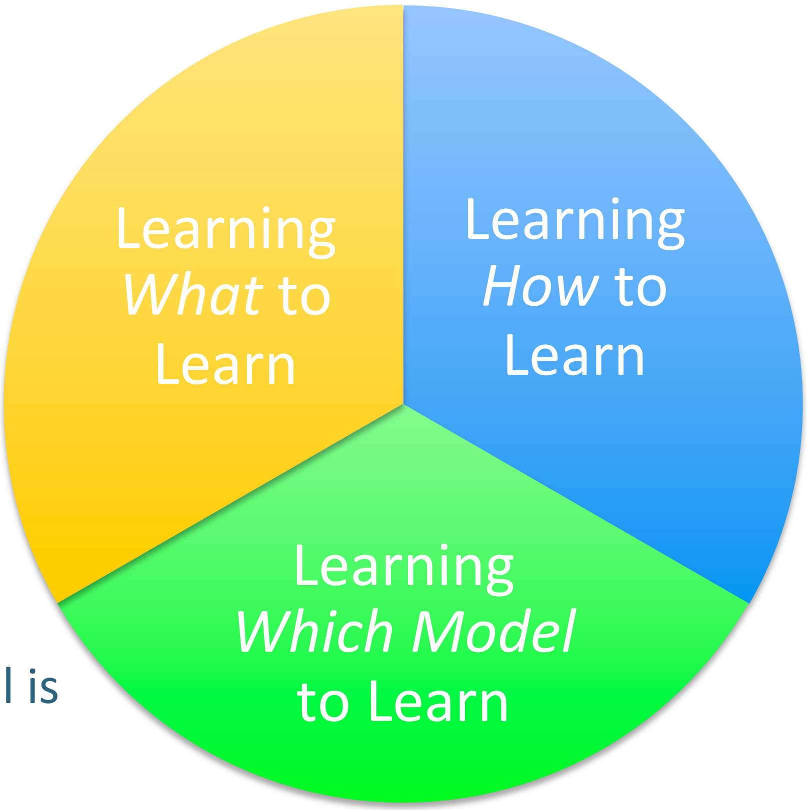

Learn which base-model is best suited for a task.

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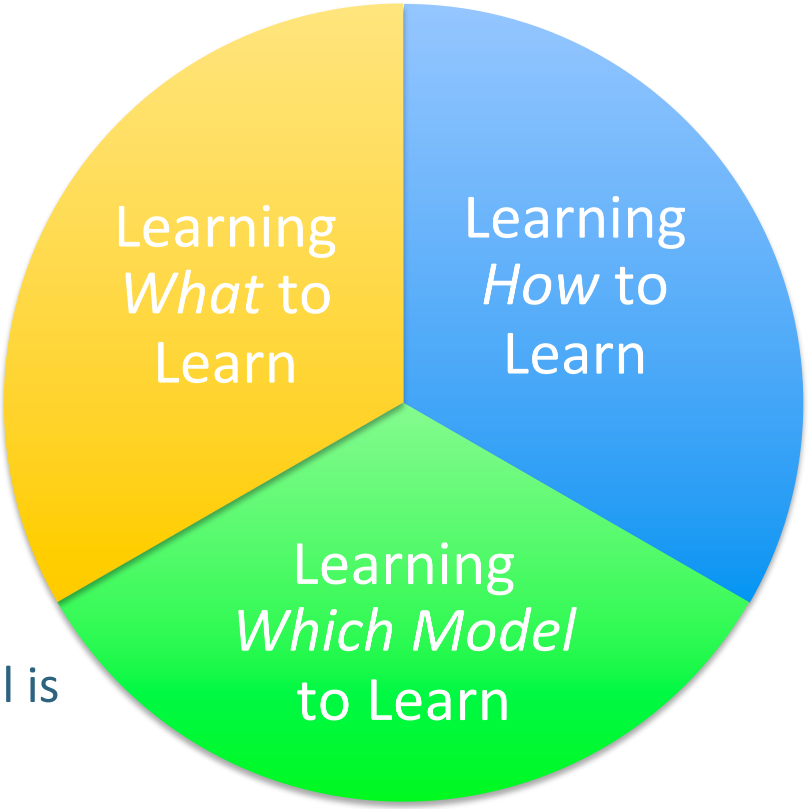

Learn which base-model is best suited for a task.

- Hyperparameter Optimization

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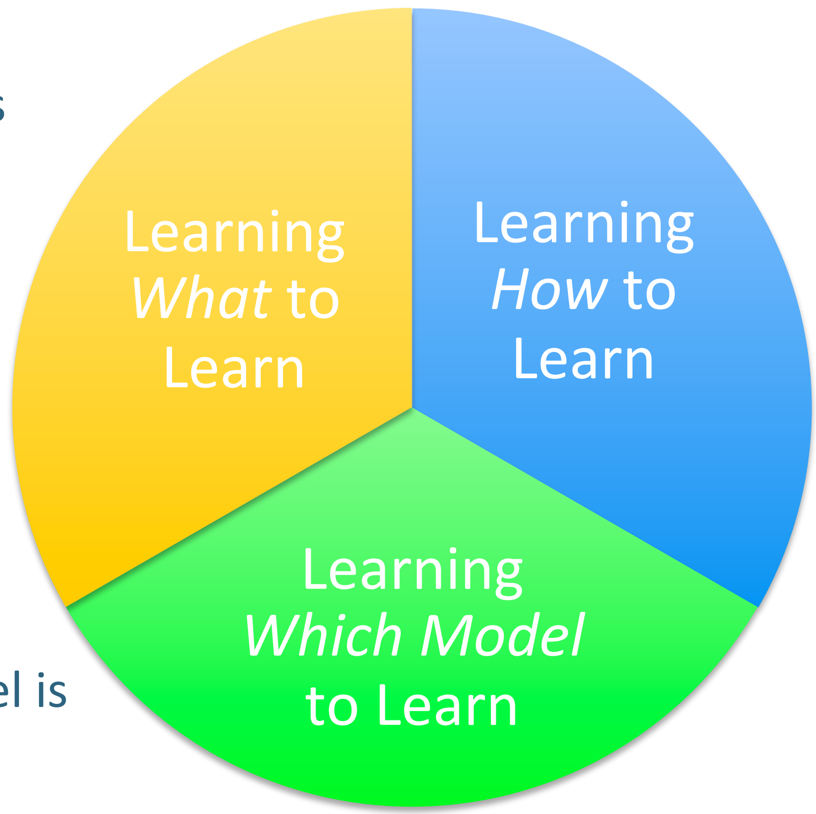

Our Contribution: Learn how to train the base-model.

Learn which base-model is best suited for a task.

- Hyperparameter Optimization

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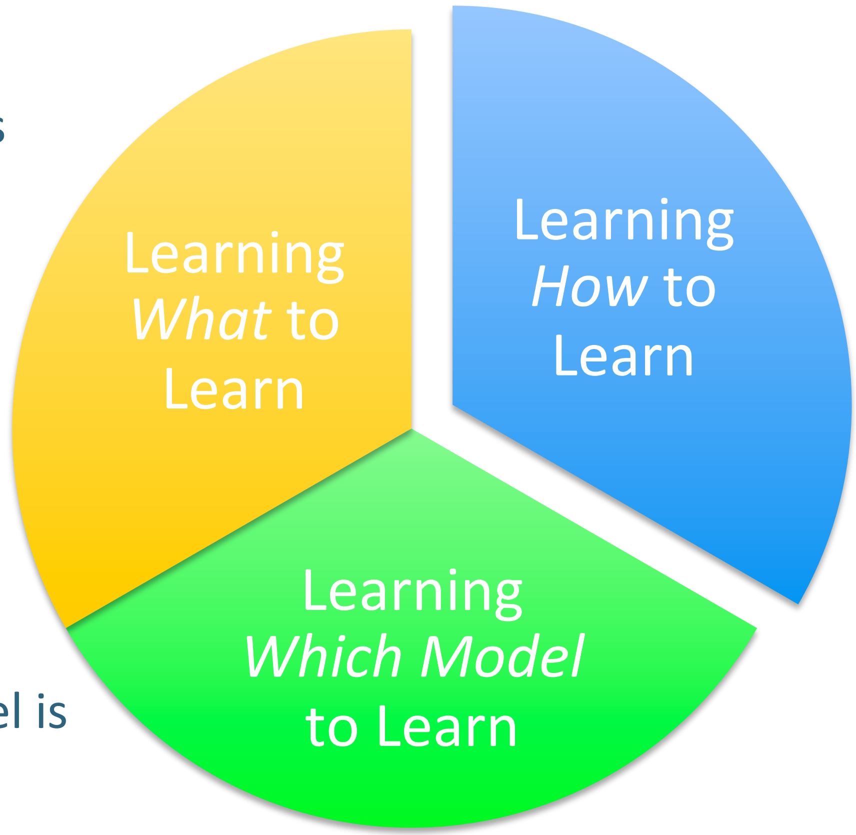

Our Contribution:
Learn how to train the base-model.
(Focus of this talk)

Learn which base-model is best suited for a task.
- Hyperparameter Optimization

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Learning How to Learn

Setting

- Most learning algorithms optimize some objective function.
  - Learning how to learn reduces to learning an optimization algorithm.
- We train an optimization algorithm on a set of objective functions.
- The learner searches the space of possible optimization algorithms and outputs an optimization algorithm that performs well on the set of objective functions.

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Learning to Optimize

Algorithm 1 General structure of optimization algorithms

Require: Objective function f
  $x^{(0)} \leftarrow$ random point in the domain of f
  for $i = 1, 2, \ldots$ **do**
    $\Delta x \leftarrow \phi(\{x^{(j)}, f(x^{(j)}), \nabla f(x^{(j)})\}_{j=0}^{i-1})$
    if stopping condition is met **then**
      return $x^{(i-1)}$
    end if
    $x^{(i)} \leftarrow x^{(i-1)} + \Delta x$
  end for

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Gradient Descent	$\phi(\cdot) = -\gamma \nabla f(x^{(i-1)})$
Momentum	$\phi(\cdot) = -\gamma \left(\sum_{j=0}^{i-1} \alpha^{i-1-j} \nabla f(x^{(j)}) \right)$

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Learned Algorithm	$\phi(\cdot) =$ Neural Net

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How do we learn $\phi(\cdot)$?

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end for

How do we learn $\phi(\cdot)$? We use reinforcement learning.

Background on Reinforcement Learning

- Set of states: $\mathcal{S} \subseteq \mathbb{R}^D$
- Set of actions: $\mathcal{A} \subseteq \mathbb{R}^d$
- Probability density over initial states: $p_i\left(s_0\right)$
- State transition probability density: $p\left(s_{t+1} \mid s_t, a_t\right)$
- Cost function: $c : \mathcal{S} \to \mathbb{R}$
- Time horizon: T
- Typically, the reinforcement learning algorithm does not know what $p\left(s_{t+1} \mid s_t, a_t\right)$ is.

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This is crucial.

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Background on Reinforcement Learning

- Policy: $\pi\left(a_t \middle| s_t, t\right)$
  - When it is independent of t, it is known as stationary.
- The goal is to find:

$$\pi^* = \arg\min_{\pi} \mathbb{E}_{s_0, a_0, s_1, \ldots, s_T}\left[\sum_{t=0}^{T} c(s_t)\right]$$

where the expectation is taken w.r.t.

$$q(s_0, a_0, s_1, \ldots, s_T) = p_i\left(s_0\right) \prod_{t=0}^{T-1} \pi\left(a_t \middle| s_t, t\right) p\left(s_{t+1} \middle| s_t, a_t\right)$$

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Reduction to Reinforcement Learning

Algorithm 1 General structure of optimization algorithms

Require: Objective function f

$x^{(0)} \leftarrow$ random point in the domain of f

for $i = 1, 2, \ldots$ **do**

$\Delta x \leftarrow \phi(\Phi(\{x^{(j)}, f(x^{(j)}), \nabla f(x^{(j)})\}_{j=0}^{i-1}))$

if stopping condition is met **then**

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Reduction to Reinforcement Learning

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en

Policy

State: $x^{(i)}$, $\Phi(\cdot)$

Action: Δx

Cost: $f(x^{(i)})$

Reduction to Reinforcement Learning

- Under this formulation, the state transition probability density $p\left(s_{t+1} \middle| s_t, a_t\right)$ captures how the gradient and objective value are likely to change for any given step vector.
  - In other words, it encodes the distribution of local geometries of the objective functions of interest.
- The geometry of an unseen objective function is unknown.
  - This is OK, since reinforcement learning does not assume knowledge of $p\left(s_{t+1} \middle| s_t, a_t\right)$.

Why Reinforcement Learning?

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Simultaneous Discovery

- A similar idea was also proposed independently by Andrychowicz et al. soon after our paper appeared:

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Learning to Optimize

Ke Li **Jitendra Malik**
Department of Electrical Engineering and Computer Sciences
University of California, Berkeley

Google DeepMind

Learning to learn by gradient descent by gradient descent

Marcin Andrychowicz **Misha Denil** **Sergio Gomez**
Matthew W. Hoffman **David Pfau** **Tom Schaul**
Nando de Freitas

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Learning to Optimize

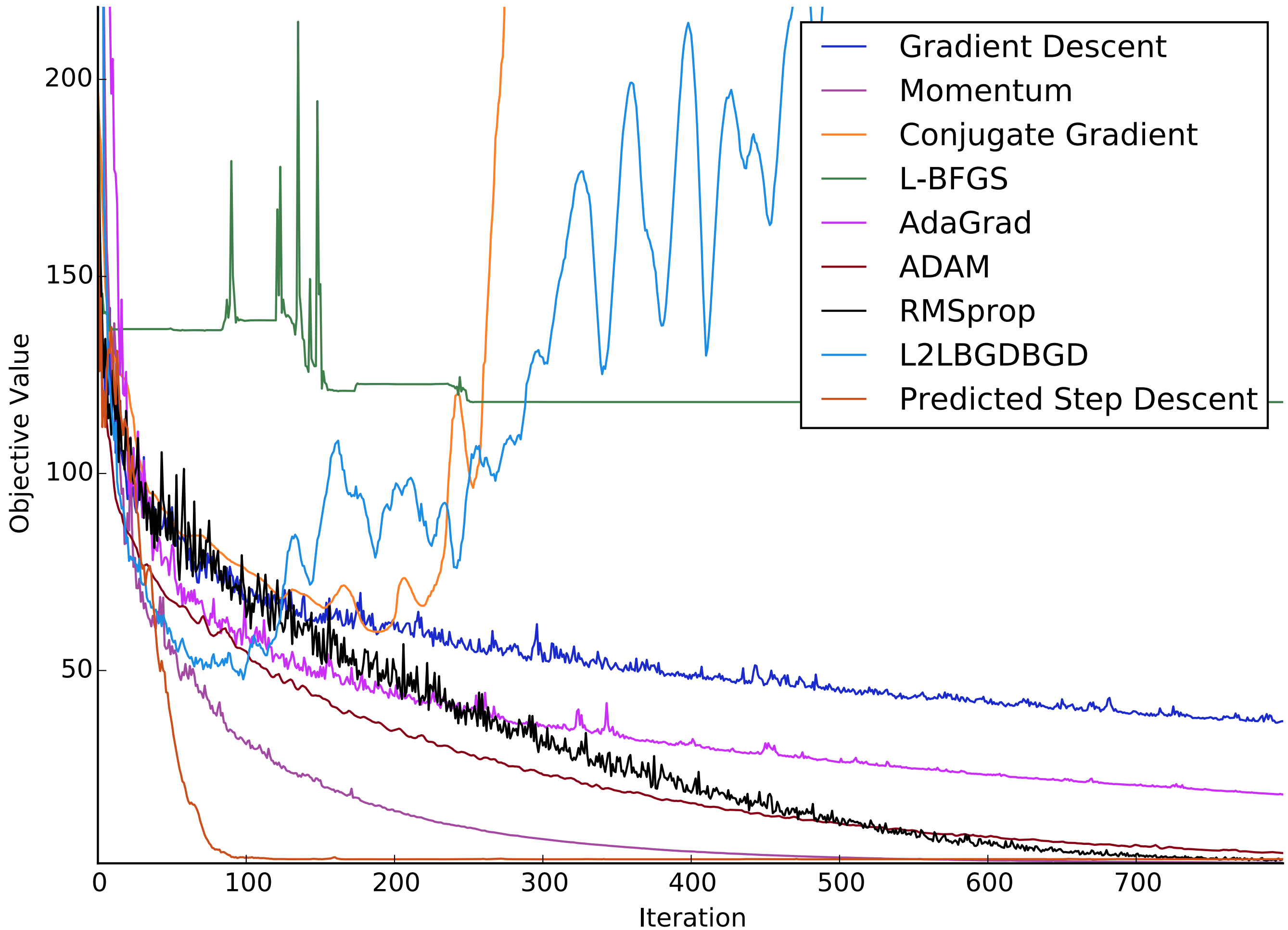
Uses Reinforcement Learning

Google DeepMind

Learning to learn by gradient descent by gradient descent

Uses Supervised Learning

Problem is Harder Than It Looks



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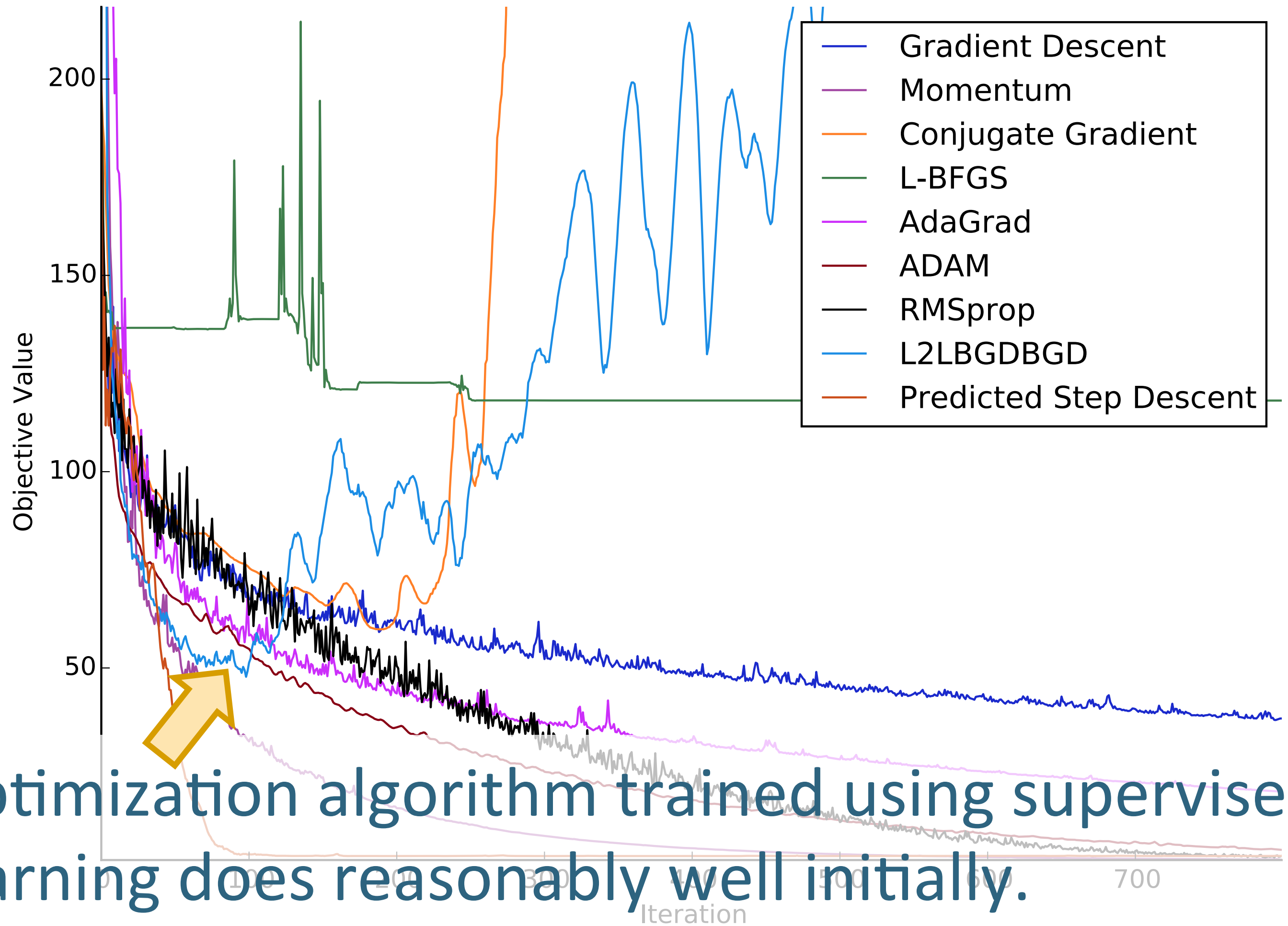

- Optimization algorithm trained using supervised learning does reasonably well initially.

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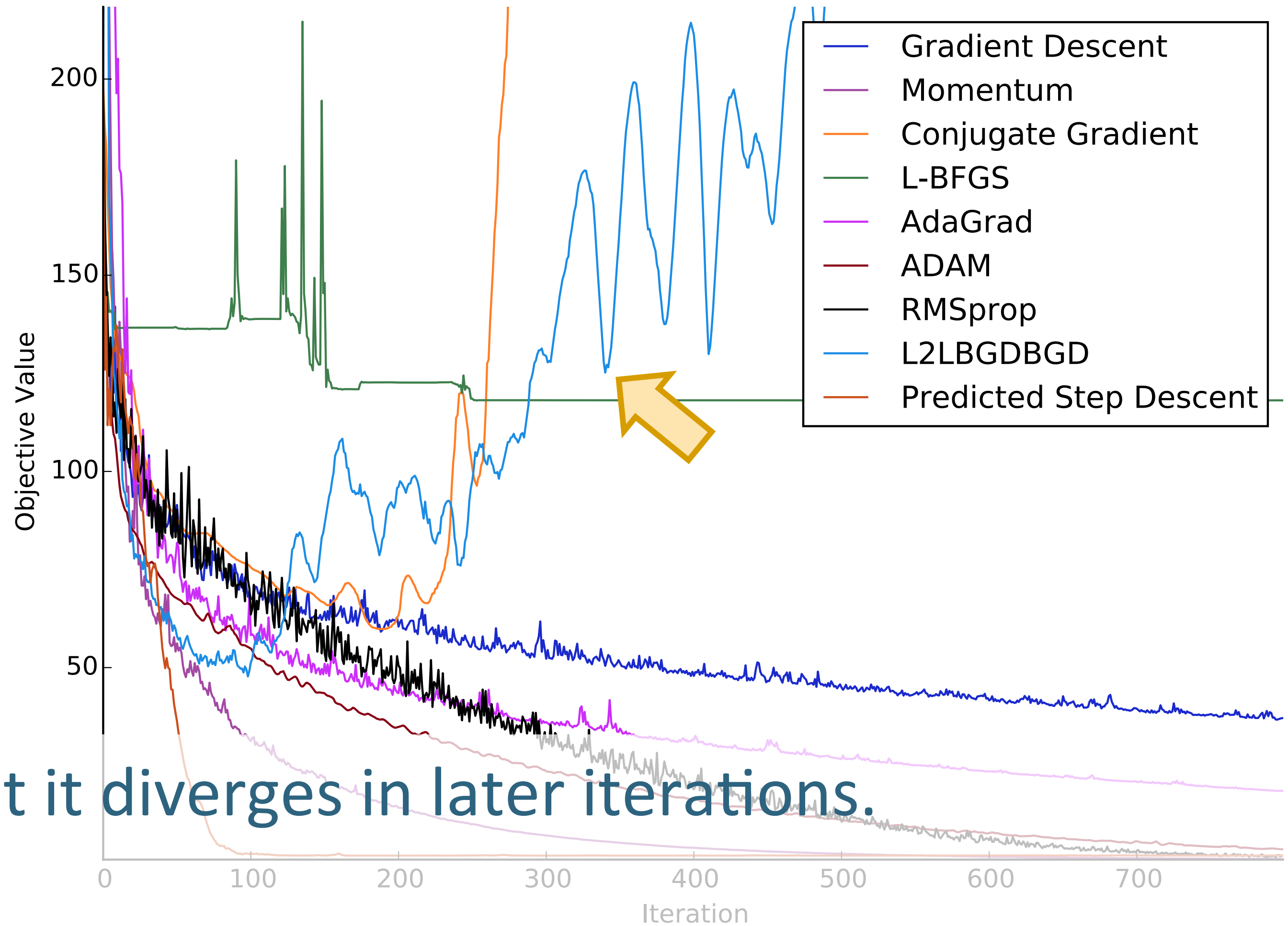
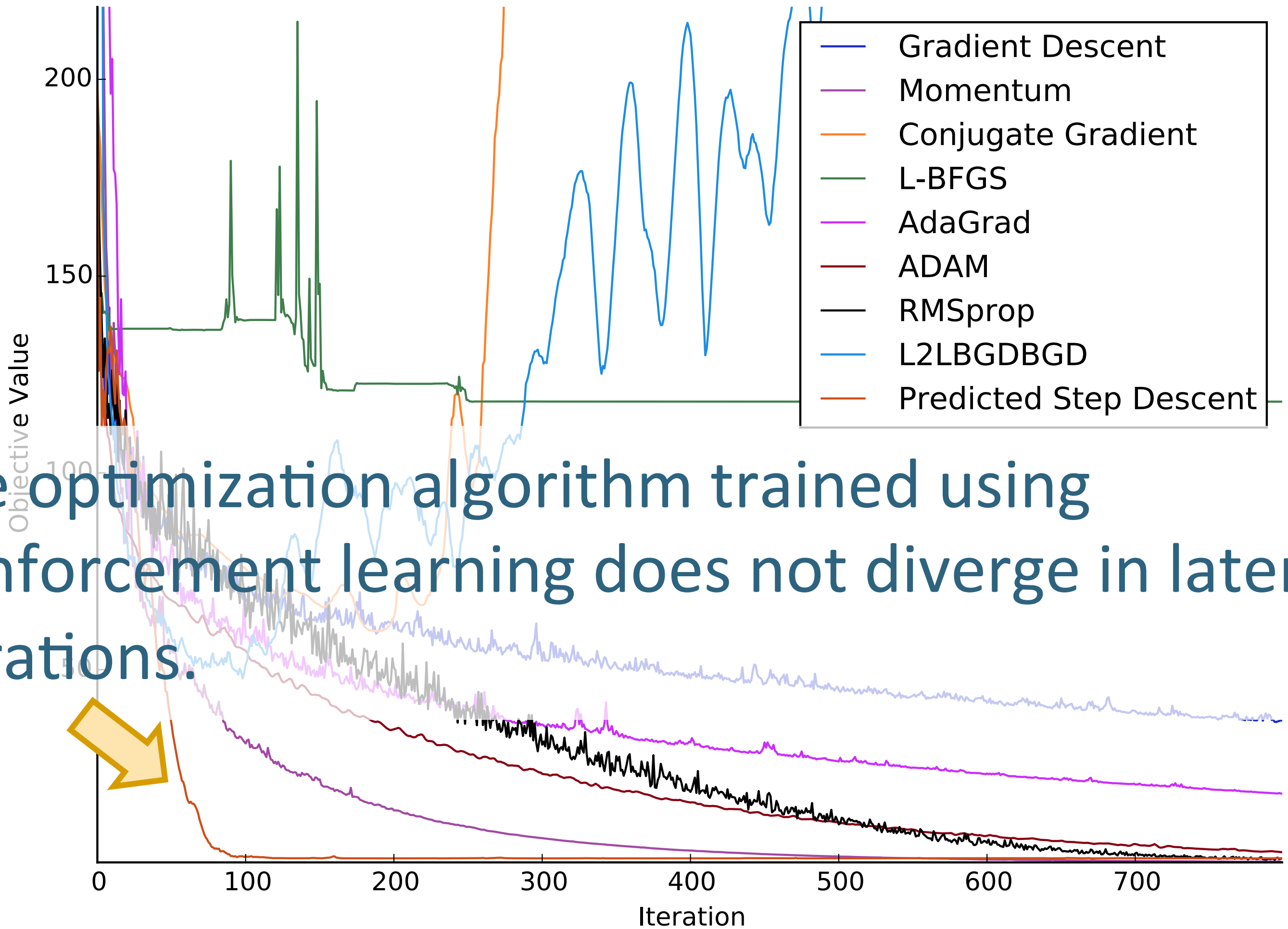
Problem is Harder Than It Looks



- But it diverges in later iterations.

Problem is Harder Than It Looks



- The optimization algorithm trained using reinforcement learning does not diverge in later iterations.

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What Generalization Means

- Each example is an objective function.
  - In the learning-to-learn setting, it is the loss function for training a base-model on a task.
  - Objective functions can differ in two ways:
    - The base-model
    - The task
- Generalization is across objective functions.
  - In the learning-to-learn setting, it is across base-models and/or tasks.
- We should train the optimization algorithm on some base-models and tasks, and test it on different base-models and tasks.

Experimental Setting

- The training set consists of one objective function: the cross-entropy loss function for training a neural net on MNIST.
- The test set consists of the loss functions for training neural nets with different architectures on different datasets, i.e.: the Toronto Faces Dataset (TFD), CIFAR-10 and CIFAR-100.
- In other words, the optimization algorithm is:
  – *Meta-trained* on the problem of training a neural net on MNIST.
  – *Meta-tested* on the problems of training neural nets on TFD, CIFAR-10 and CIFAR-100.

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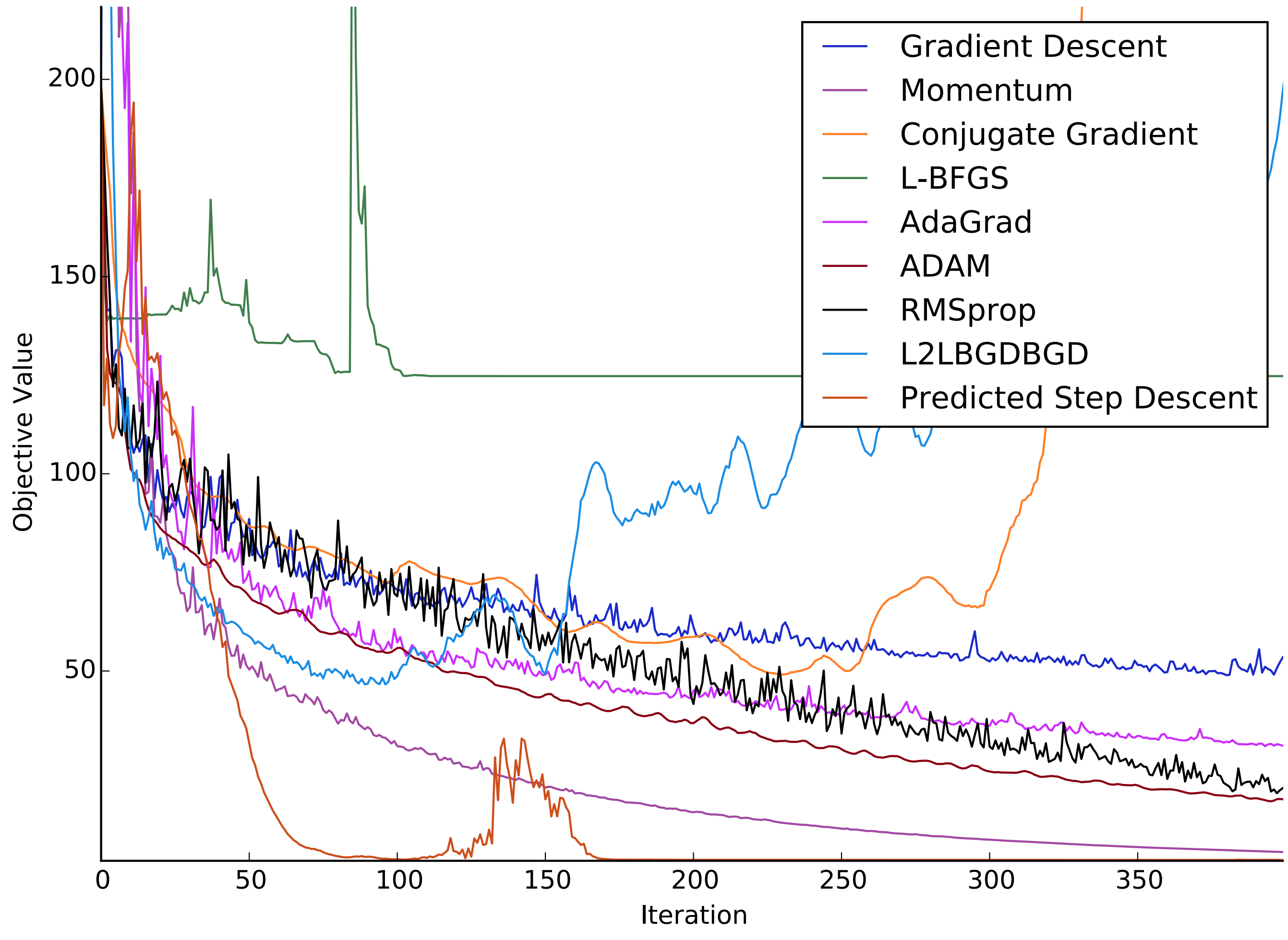
Larger Architecture (TFD)



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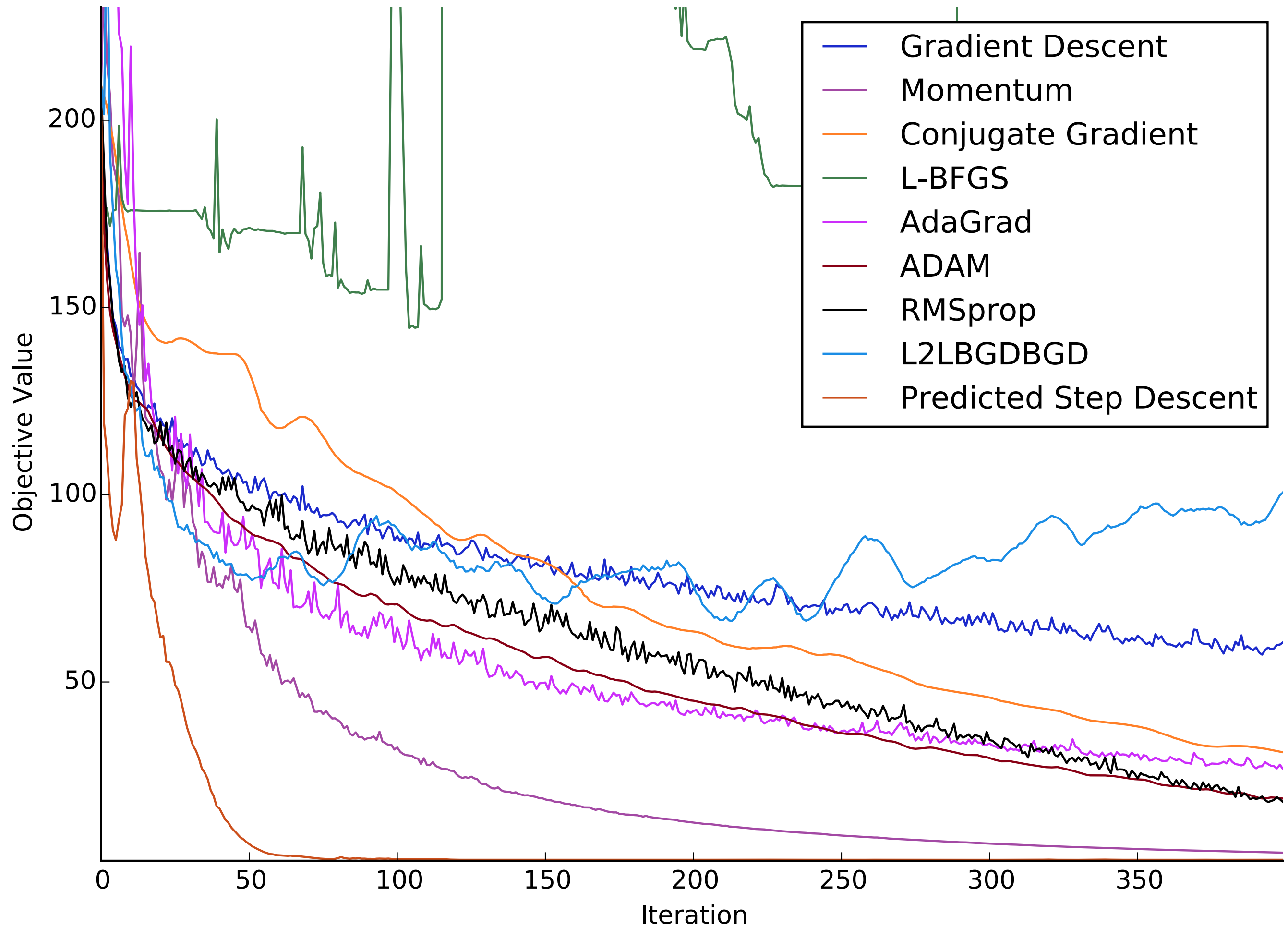
Larger Architecture (CIFAR-10)



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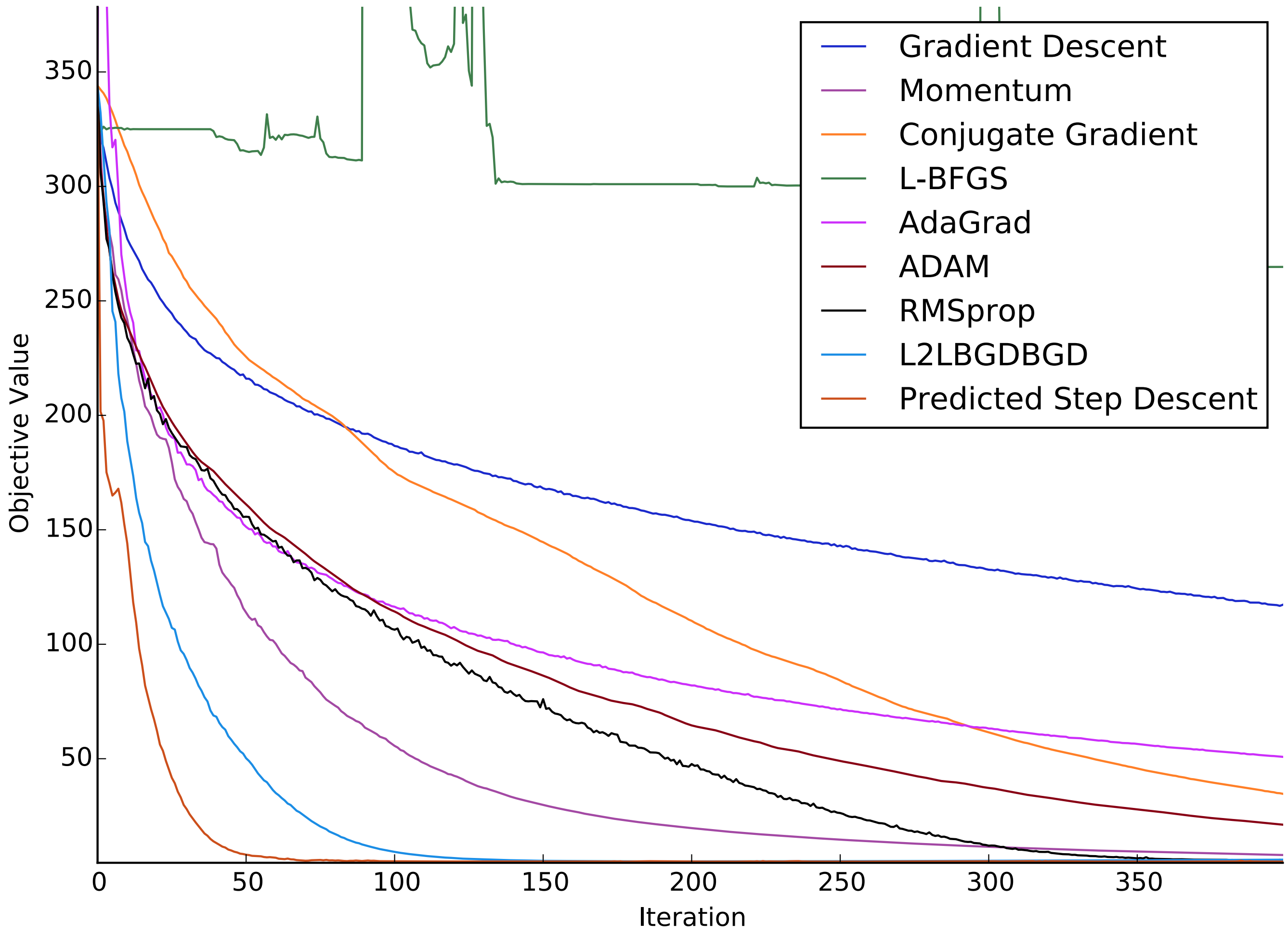
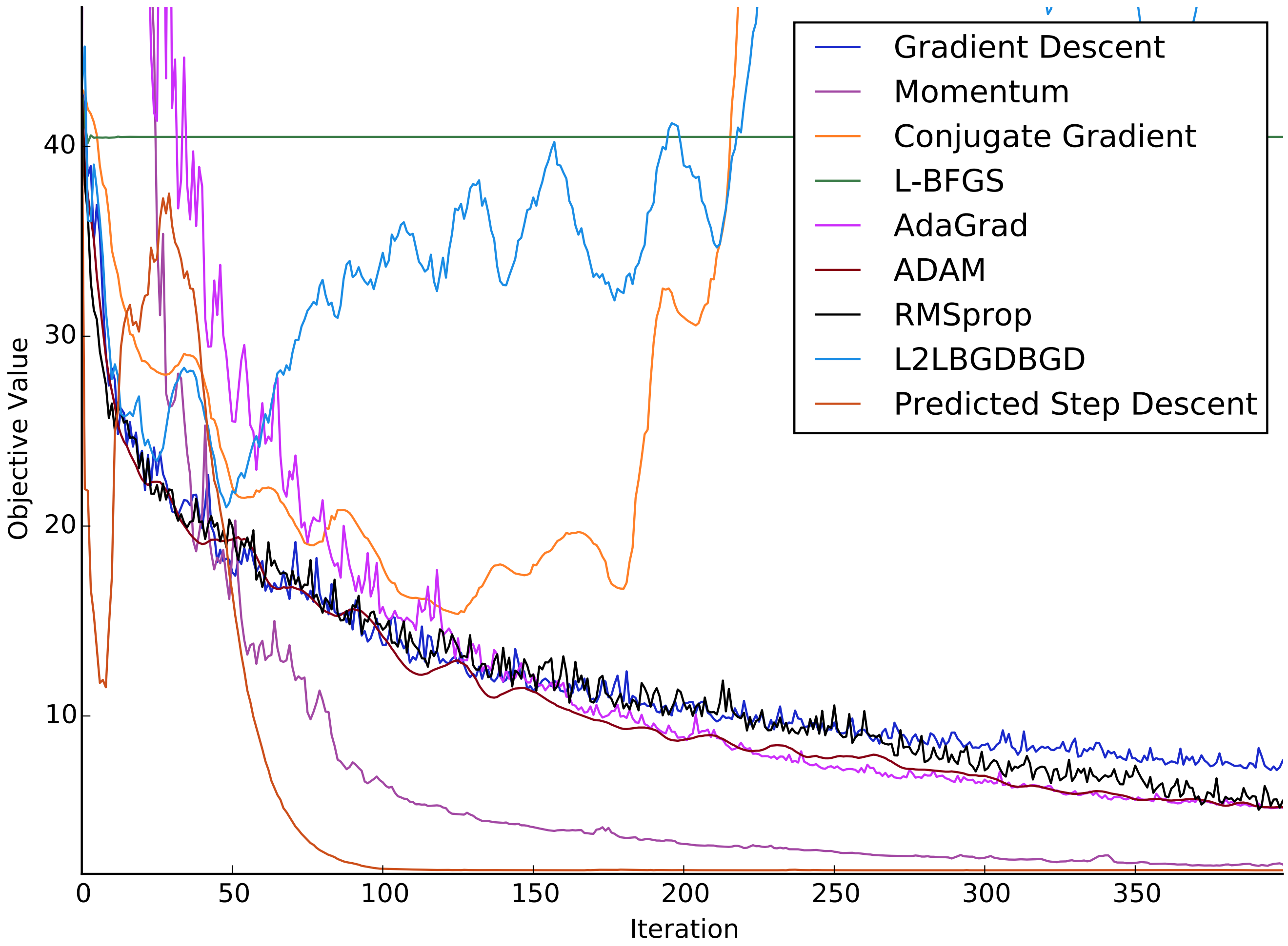
Larger Architecture (CIFAR-100)



Noisier Gradients (TFD)



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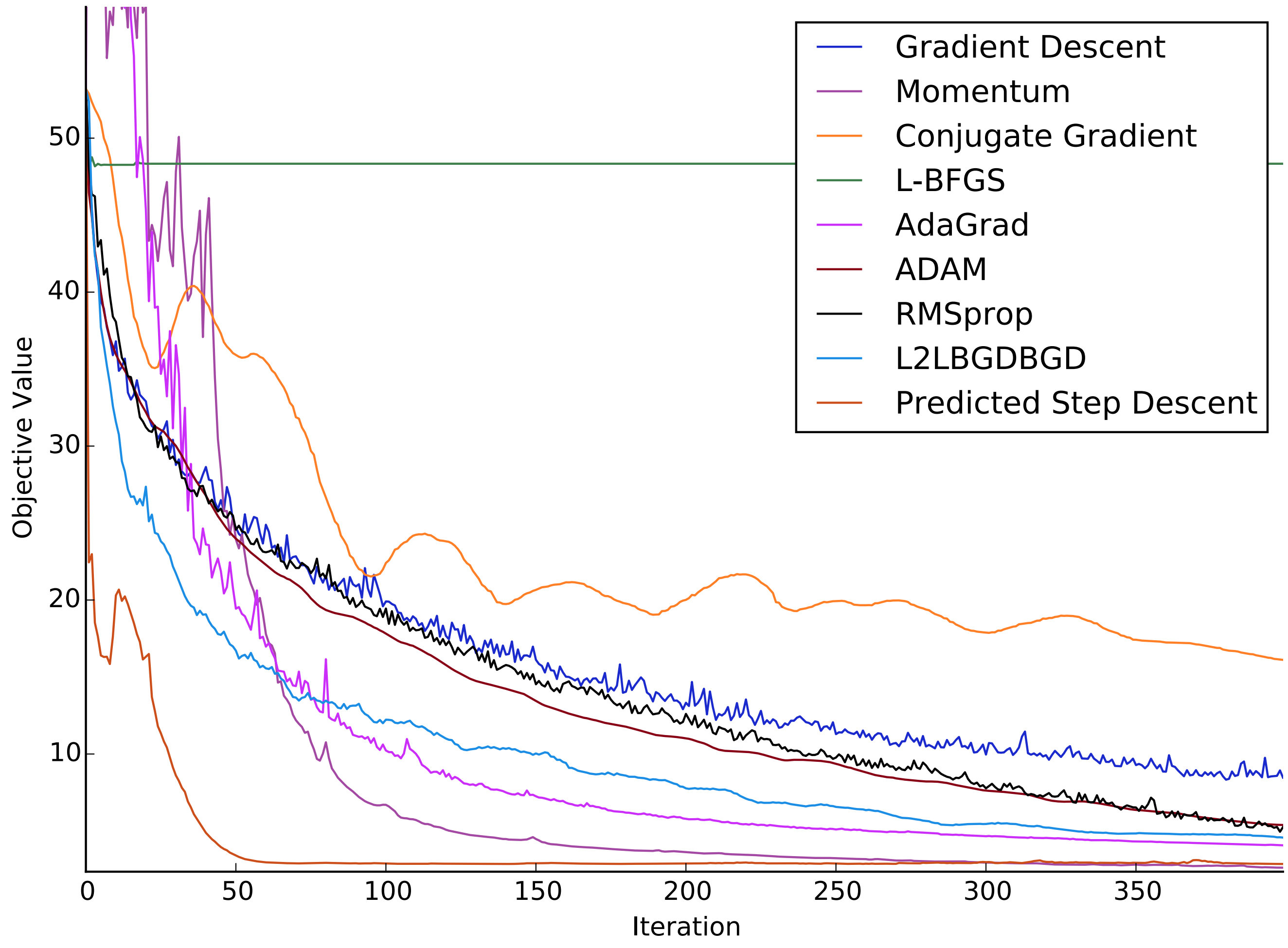
Noisier Gradients (CIFAR-10)



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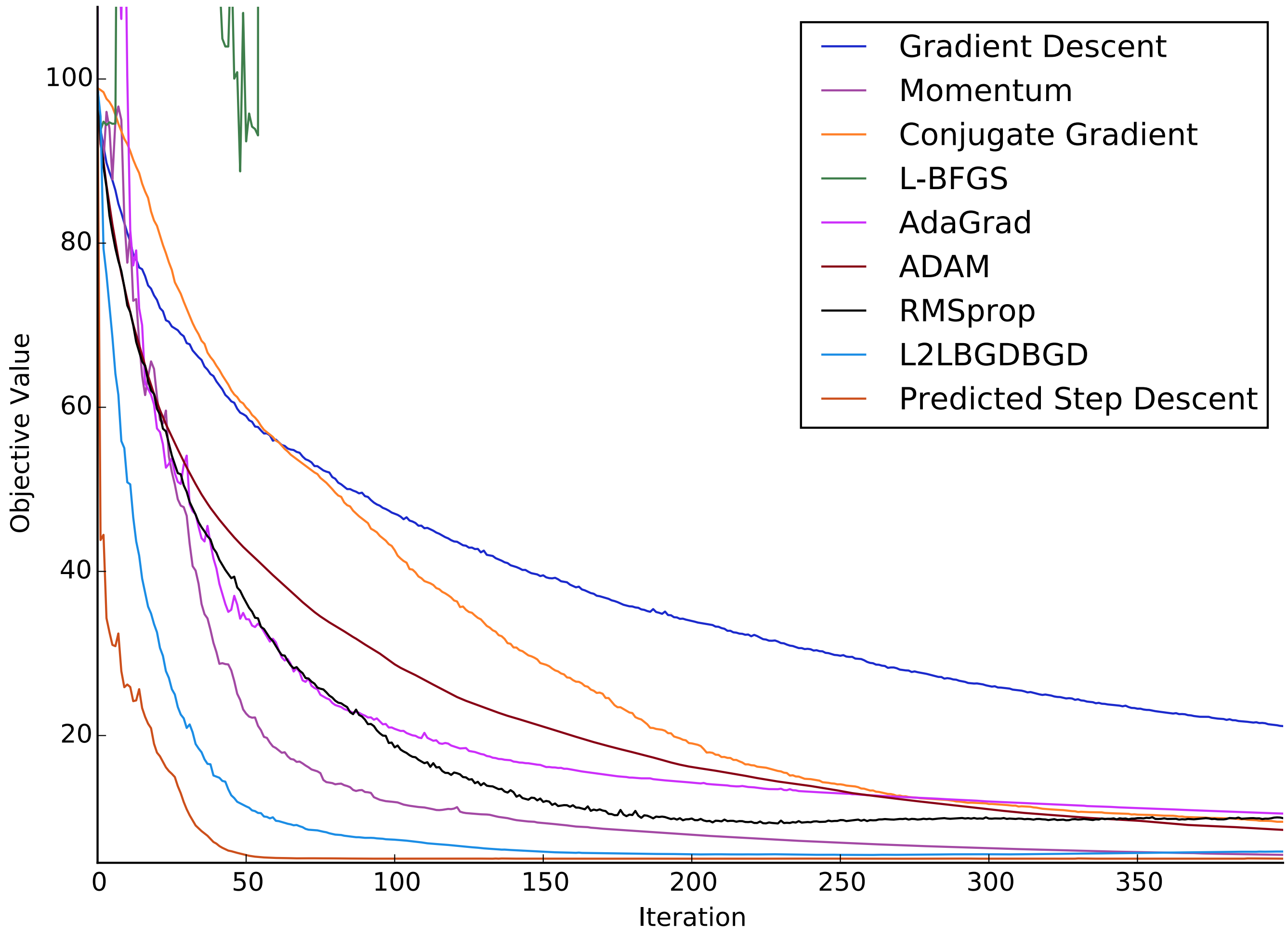
Noisier Gradients (CIFAR-100)



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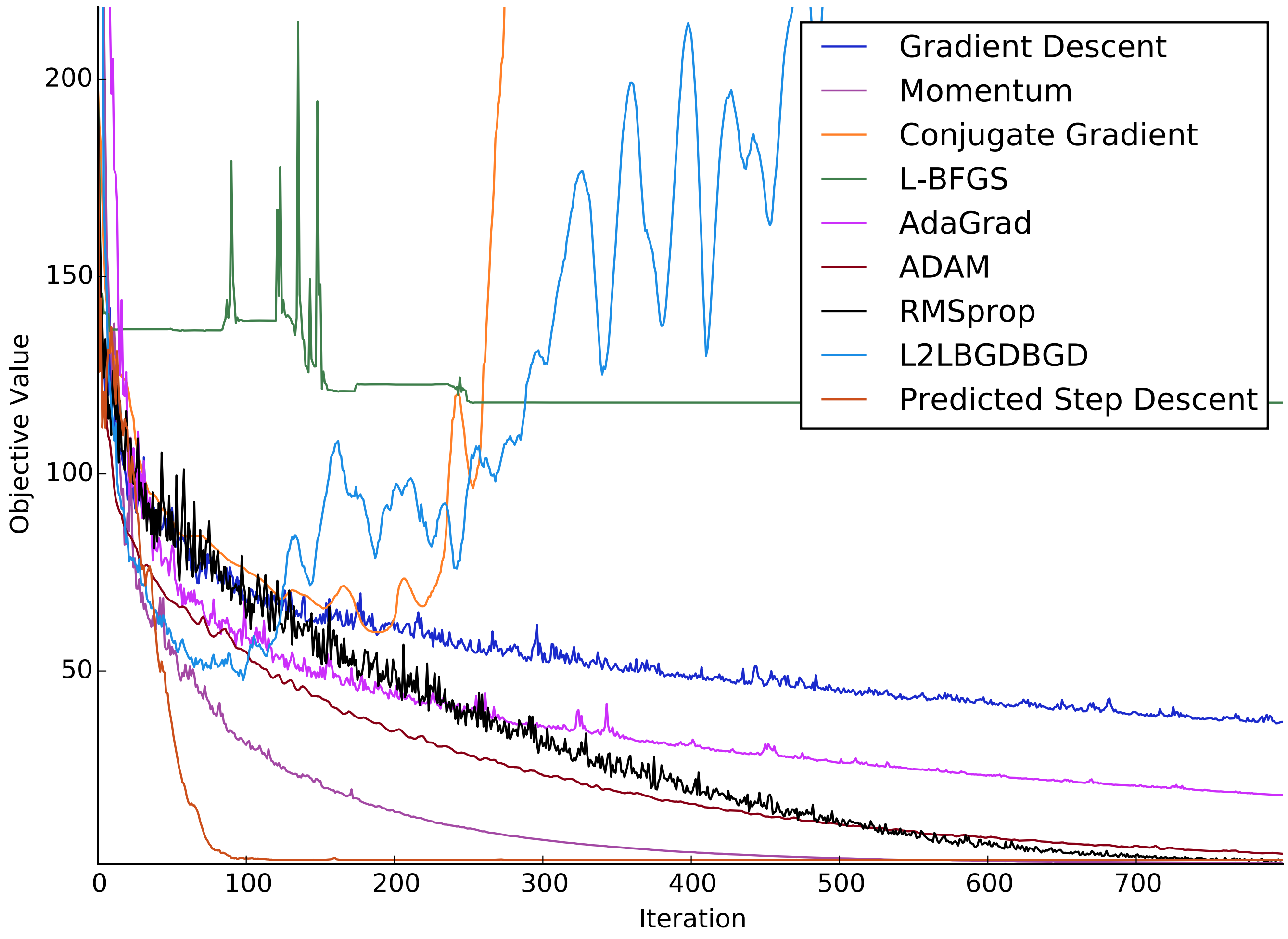
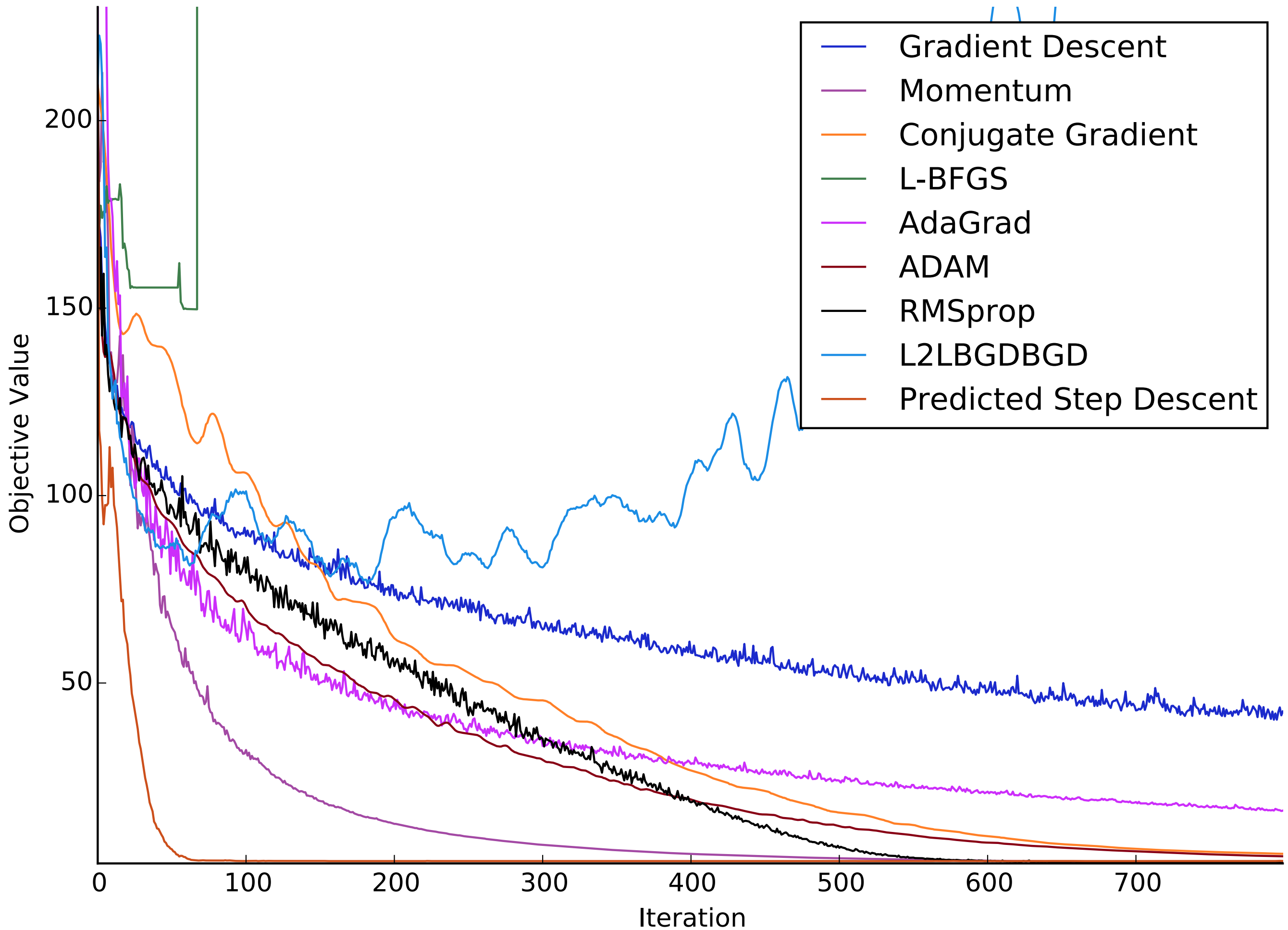
Longer Time Horizon (TFD)



Longer Time Horizon (CIFAR-10)



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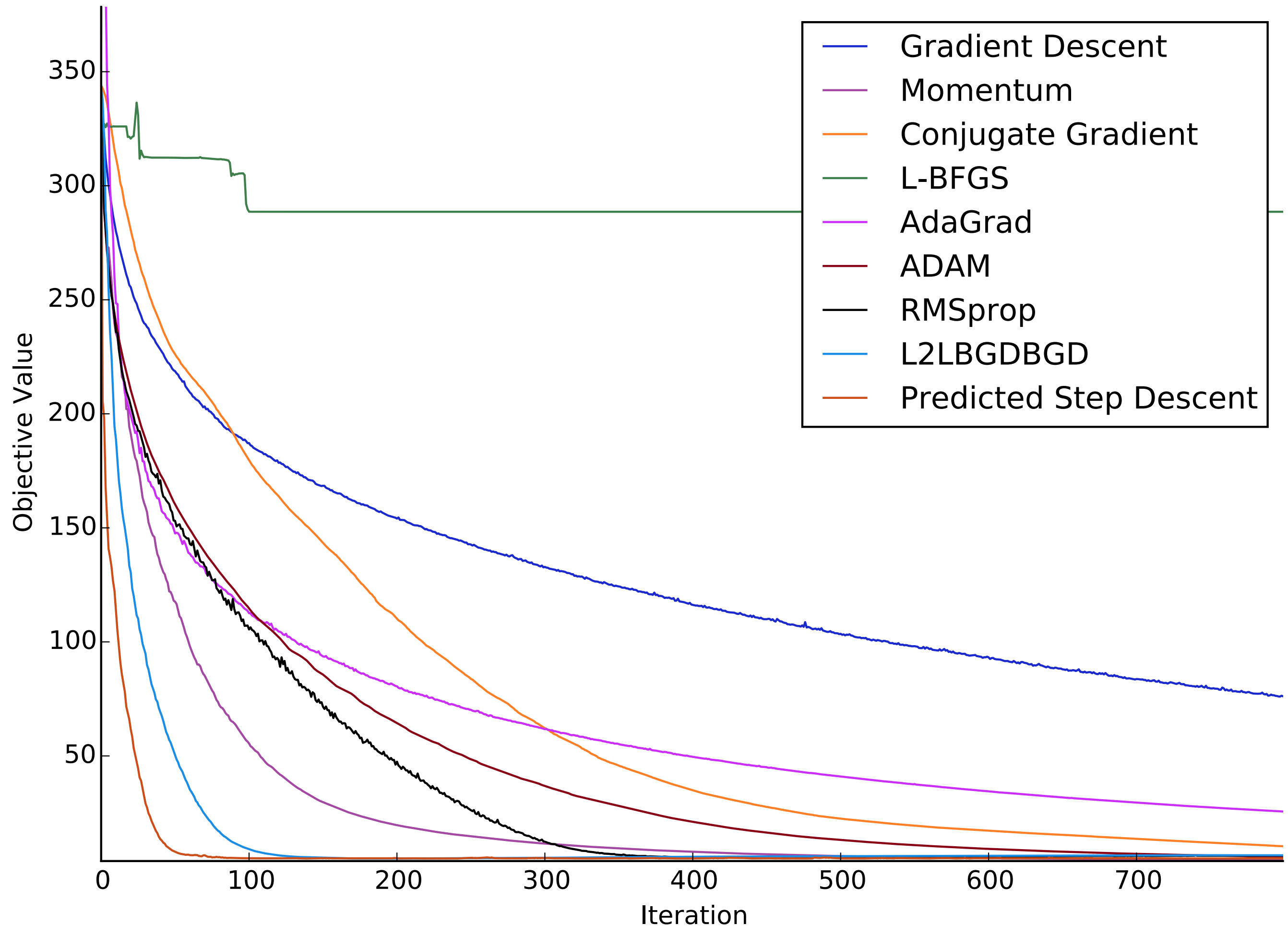
Longer Time Horizon (CIFAR-100)



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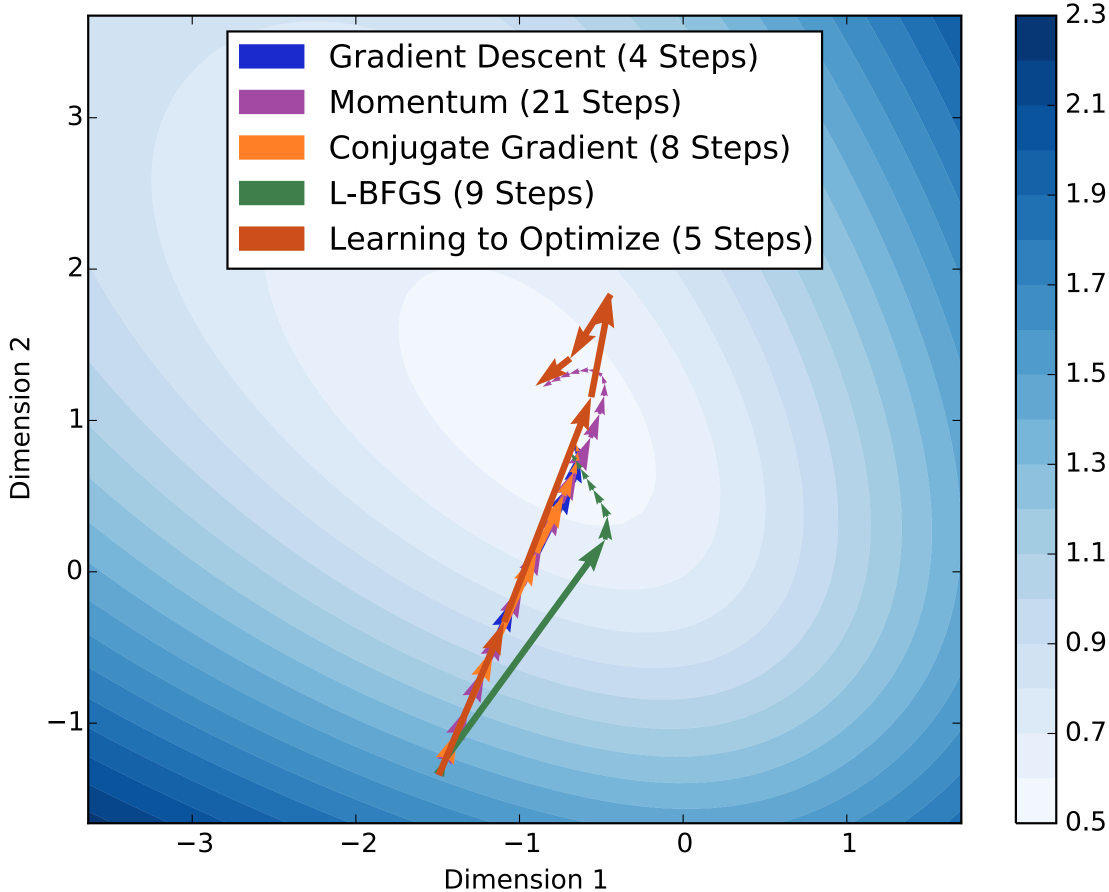
2D Logistic Regression



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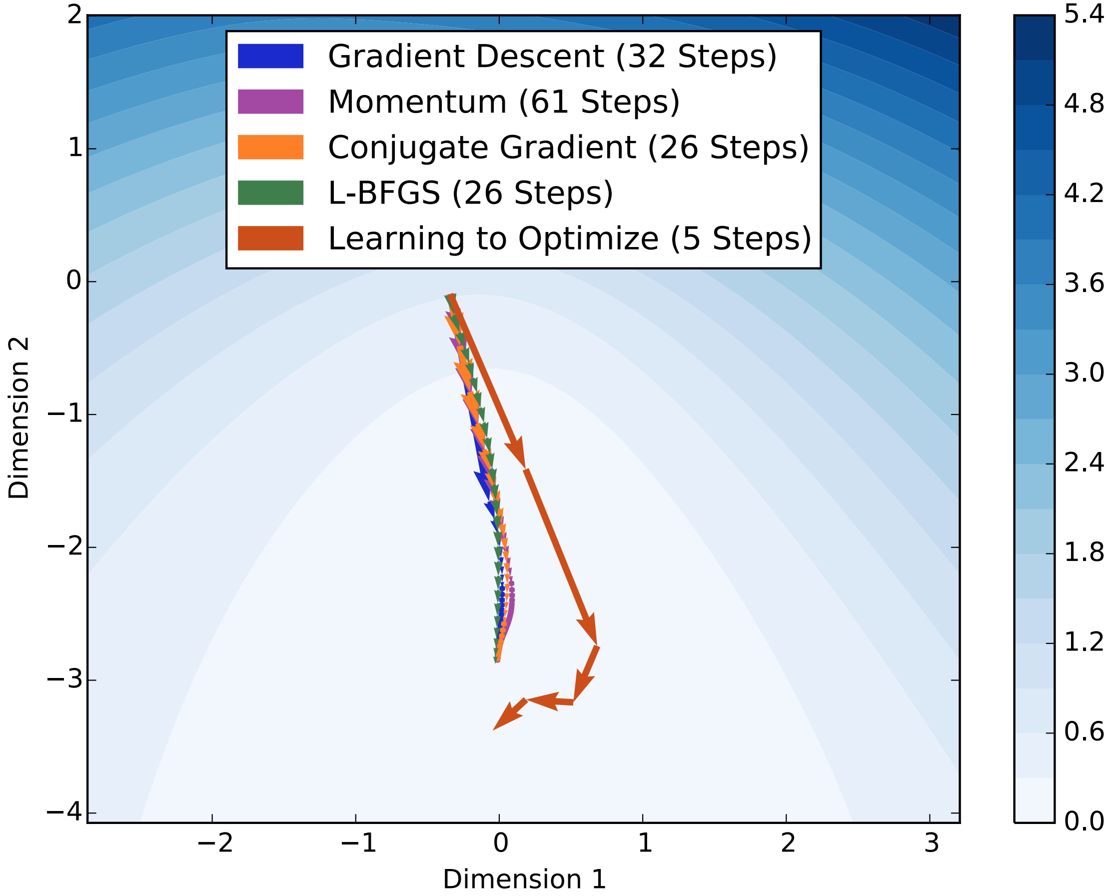

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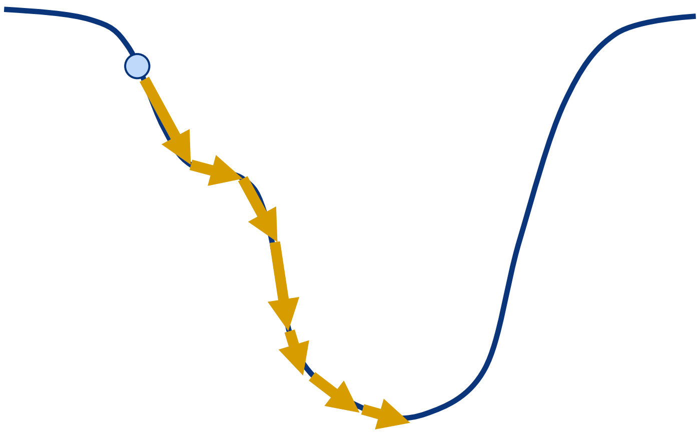
Generalization

Importance of Generalization

- Suppose we evaluate the performance of the optimizer on the training set.
- To learn an optimizer, we can simply run a traditional optimizer and memorize the solution.
- This is the best optimizer, since it gets to the optimum in one step.



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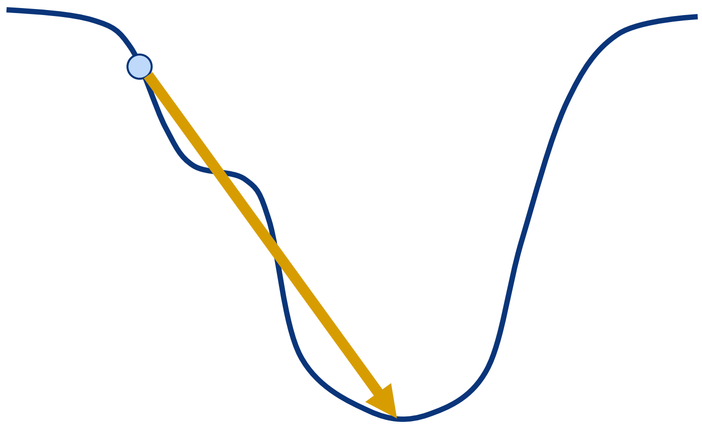

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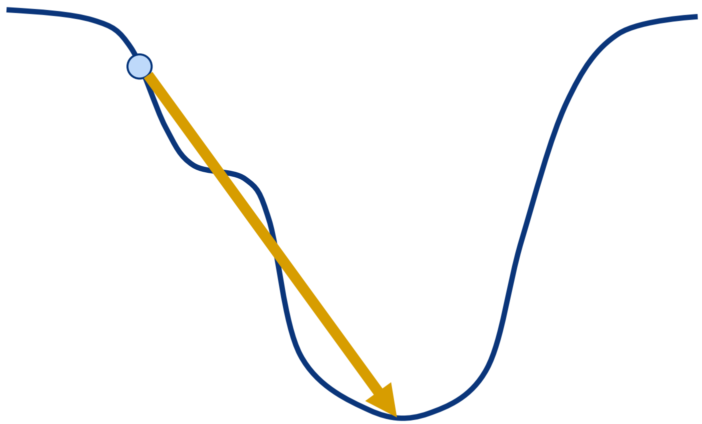

It would be pointless to learn the optimizer if we didn't care about generalization.

Extent of Generalization

- Generalization to *similar* base-models on *similar* tasks
  - Learned optimizer could memorize parts of the optimal parameters that are common across tasks and base-models.
    - E.g.: Weights of the lower layers in neural nets
  - Essentially the same as learning *what* to learn.

Extent of Generalization

- Stronger notion: Generalization to *similar* base-models on *dissimilar* tasks
  - The optimal parameters for dissimilar tasks are likely completely different.
  - An optimizer that memorizes any part of the optimal parameters will fail.
  - An optimizer that works in this setting must have learned not what the optimum is, but how to find it.

Extent of Generalization

- Even stronger notion: Generalization to *dissimilar* base-models on *dissimilar* tasks
  - The objective functions at test time could be arbitrarily different from the objective functions seen during training.
  - This is impossible – there is no optimizer that works well on all possible objective functions.

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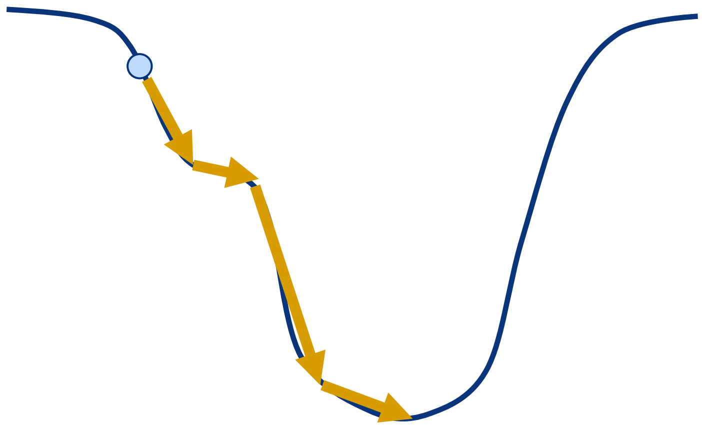
Extent of Generalization

- Given any optimizer, we can always find an objective function that it performs poorly on.
- We can simply change the objective function so that the final objective value is large.



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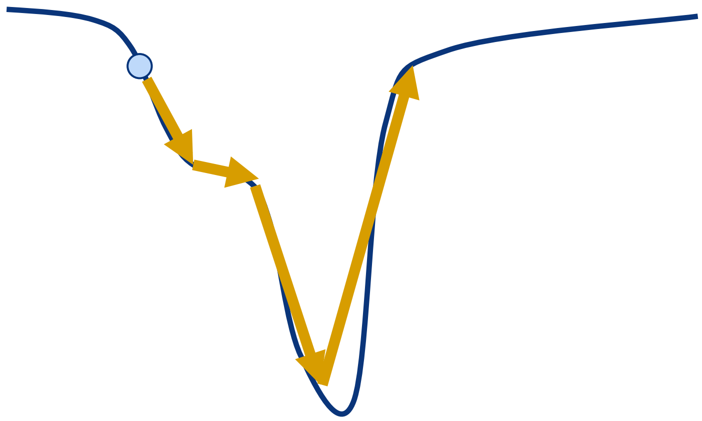

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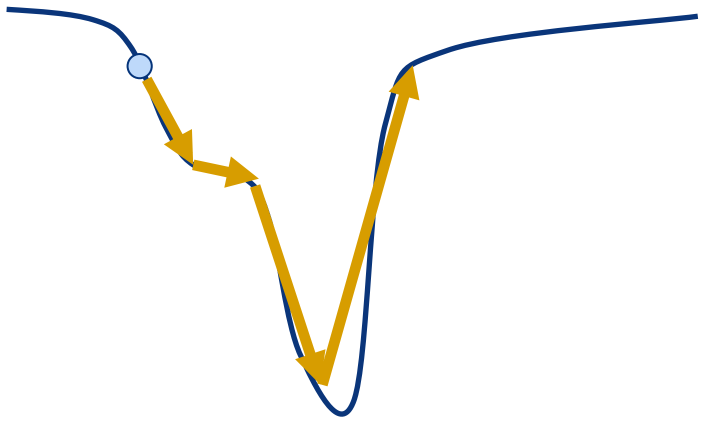

It is not possible for the learned optimizer to generalize to all possible objective functions.

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Problem of Supervised Learning

- Supervised learning requires one of the following:
  – Observations at each time step are i.i.d., or
  – The dependence of the future observation on the current observation is known.
- In our setting, neither is true:
  – The step the optimizer takes affects future gradients.
  – How the current step affects the next gradient, i.e. the local geometry, is not known at test time.

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Problem of Supervised Learning

- When backpropagating through time, supervised learning essentially assumes the local geometry of an unseen objective function is the same as the local geometry of *one* of the training objective functions at *all* time steps.
  - In other words, it assumes $p\left(s_{t+1} \left| s_t, a_t \right.\right)$ is known and models it using the Hessians of the training objective functions.
  - This is incorrect, since the Hessians of an unseen objective function will be different.
- Hence, supervised learning overfits to the geometries of training objective functions.

Problem of Supervised Learning

- When an optimizer trained with supervised learning is applied to an unseen objective function:
  - It takes a step,

    → sees an unexpected gradient at the next iteration,

    → takes a step that is slightly off,

    → finds out the next gradient is even more unexpected,

    → takes another step that is more off,

    …

    → eventually diverges.

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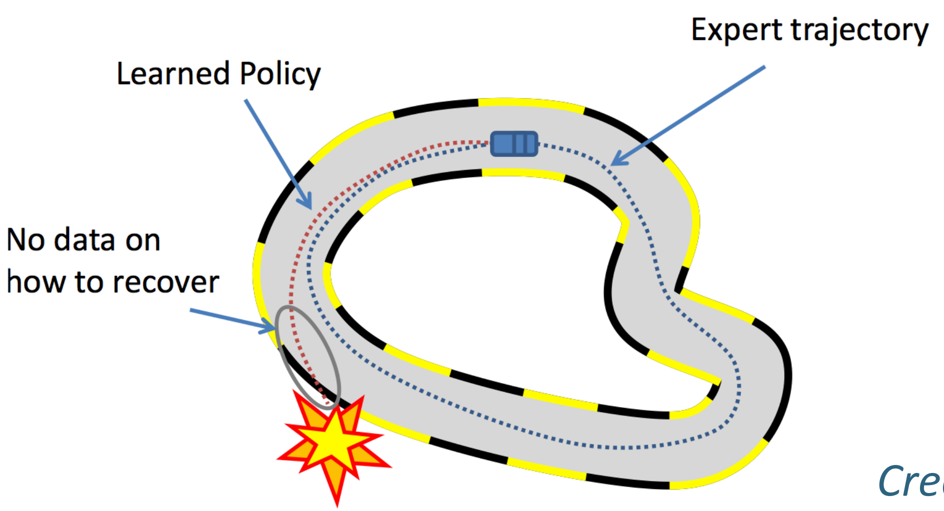
Problem of Supervised Learning

- This is known as the problem of compounding errors.
  - Supervised learning leads to a cumulative error that grows quadratically in the time horizon, rather than linearly. (Ross & Bagnell, 2010)



Credit: John Schulman

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Why RL Solves This Problem

- Reinforcement learning algorithm does not assume knowledge of $p\left(s_{t+1} \mid s_t, a_t\right)$, which characterizes the geometries of training objective functions.
  - So, conditions at meta-training and meta-test times match.
  - The learned policy must account for the uncertainty in $p\left(s_{t+1} \mid s_t, a_t\right)$, and must know how to recover from mistakes.

Reinforcement Learning Method

Guided Policy Search

- An (approximate) policy search algorithm for continuous state and action spaces. (Levine et al., 2015)
- Maintains two policies, ψ and π .
  - ψ lies in a time-varying linear policy class.
    - Optimal policy can be found in closed form.
  - π lies in a stationary non-linear policy class.
- Alternates between solving for ψ and π .

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ADMM

- Alternating direction method of multipliers (Boyd et al., 2011) solves the following problem:

$$\min_{\theta \in \Theta, \eta \in H} f(\theta) + g(\eta) \text{ s.t. } A\theta + B\eta = c$$

where f and g are convex functions, and Θ and H are closed convex sets.

- It alternates between the following updates:

$$\theta^{(t+1)} \leftarrow \arg\min_{\theta \in \Theta} f(\theta) + \langle \lambda^{(t)}, A\theta + B\eta^{(t)} - c \rangle + \frac{\rho}{2} \left\| A\theta + B\eta^{(t)} - c \right\|_2^2$$

$$\eta^{(t+1)} \leftarrow \arg\min_{\eta \in H} g(\eta) + \langle \lambda^{(t)}, A\theta^{(t+1)} + B\eta - c \rangle + \frac{\rho}{2} \left\| A\theta^{(t+1)} + B\eta - c \right\|_2^2$$

$$\lambda^{(t+1)} \leftarrow \lambda^{(t)} + \rho \left(A\theta^{(t+1)} + B\eta^{(t+1)} - c \right)$$

Bregman ADMM

- Bregman ADMM (Wang & Banerjee, 2014) generalizes ADMM and uses Bregman divergence as penalty. It solves:

$$\min_{\theta\in\Theta,\eta\in H} f(\theta) + g(\eta) \text{ s.t. } A\theta + B\eta = c$$

  where f and g are convex functions, and Θ and H are closed convex sets.
- It alternates between the following updates:

$$\theta^{(t+1)} \leftarrow \arg\min_{\theta\in\Theta} f(\theta) + \langle \lambda^{(t)}, A\theta + B\eta^{(t)} - c\rangle + \boxed{\rho B_\phi(c - A\theta, B\eta^{(t)})}$$

$$\eta^{(t+1)} \leftarrow \arg\min_{\eta\in H} g(\eta) + \langle \lambda^{(t)}, A\theta^{(t+1)} + B\eta - c\rangle + \boxed{\rho B_\phi(B\eta, c - A\theta^{(t+1)})}$$

$$\lambda^{(t+1)} \leftarrow \lambda^{(t)} + \rho\left(A\theta^{(t+1)} + B\eta^{(t+1)} - c\right)$$

Reinforcement Learning Problem

- Recall the reinforcement learning problem:

$$\min_{\theta} \mathbb{E}_{s_0, a_0, s_1, \ldots, s_T} \left[\sum_{t=0}^{T} c(s_t) \right]$$

where the expectation is taken w.r.t.

$$q(s_0, a_0, s_1, \ldots, s_T) = p_i(s_0) \prod_{t=0}^{T-1} \pi(a_t | s_t; \theta) \, p(s_{t+1} | s_t, a_t)$$

State | Action | Initial State Distribution | Policy | Policy Parameters | State Transition Distribution

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Reinforcement Learning Problem

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State

Action

Initial State Distribution

Policy

Policy Parameters

State Transition Distribution

Guided Policy Search

- Guided Policy Search performs dual decomposition:

$$\min_{\theta,\eta} \mathbb{E}_{\psi}\left[\sum_{t=0}^{T} c(s_t)\right] \text{ s.t. } \psi\left(a_t \middle| s_t, t; \eta\right) = \pi\left(a_t \middle| s_t; \theta\right) \ \forall a_t, s_t, t$$

- It relaxes the problem by only enforcing equality on the first moments*:

$$\min_{\theta,\eta} \mathbb{E}_{\psi}\left[\sum_{t=0}^{T} c(s_t)\right] \text{ s.t. } \mathbb{E}_{\psi}\left[a_t\right] = \mathbb{E}_{\psi}\left[\mathbb{E}_{\pi}\left[a_t \middle| s_t\right]\right] \ \forall t$$

*The Bregman divergence penalty is applied on the original distributions.

Guided Policy Search

- To solve the problem, it uses Bregman ADMM, which alternates between the following updates:

$$\eta \leftarrow \arg\min_{\eta} \sum_{t=0}^{T} \mathbb{E}_{\psi}\left[c(s_t) - \lambda_t^T a_t\right] + \nu_t \mathbb{E}_{\psi}\left[D_{KL}\left(\psi\left(a_t \middle| s_t, t; \eta\right) \middle\| \pi\left(a_t \middle| s_t; \theta\right)\right)\right]$$

$$\theta \leftarrow \arg\min_{\theta} \sum_{t=0}^{T} \lambda_t^T \mathbb{E}_{\psi}\left[\mathbb{E}_{\pi}\left[a_t \middle| s_t\right]\right] + \nu_t \mathbb{E}_{\psi}\left[D_{KL}\left(\pi\left(a_t \middle| s_t; \theta\right) \middle\| \psi\left(a_t \middle| s_t, t; \eta\right)\right)\right]$$

$$\lambda_t \leftarrow \lambda_t + \alpha \nu_t \left(\mathbb{E}_{\psi}\left[\mathbb{E}_{\pi}\left[a_t \middle| s_t\right]\right] - \mathbb{E}_{\psi}\left[a_t\right]\right) \ \forall t$$

- The optimization in the first update can be solved in closed form using a modification of linear-quadratic regulator (LQR).

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Landscape of Meta-Learning Methods

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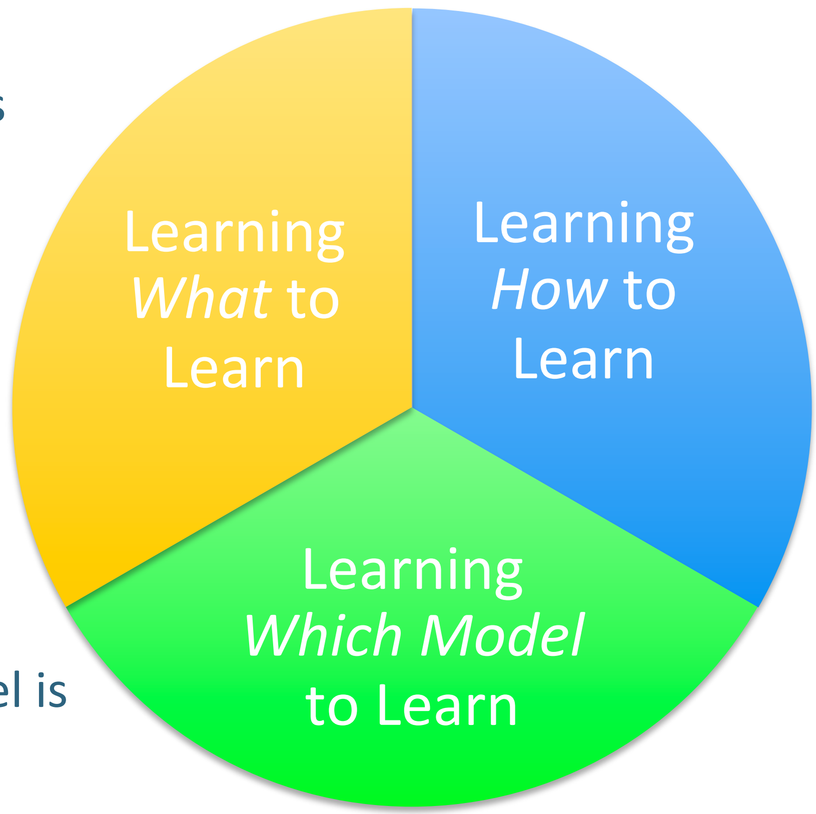
Forms of Learning to Learn

Learn parameter values of the base-model that are useful across tasks.

- Transfer Learning
- Multi-Task Learning
- Few-Shot Learning



Learn how to train the base-model.

Learn which base-model is best suited for a task.

- Hyperparameter Optimization

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Learning *What* to Learn

Goal	• Learn what parameter values of the base-model are useful across tasks.
Meta-knowledge	• Intermediate features that are shared by tasks across the family, e.g. Gabor filters for vision tasks.
Extent of Generalization	• Need to generalize across *similar* tasks.
Parameterization Challenges	• Need to parameterize the space of intermediate features – this is straightforward.
Examples	• Transfer & multi-task learning, e.g. (Suddarth & Kergosien, 1990) • Few-shot learning, e.g. (Finn et al., 2017), (Snell et al., 2017)

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Learning *Which Model* to Learn

Goal	• Learn which base-model is best suited for a task.
Meta-knowledge	• Correlations between different base-models and their performance on different tasks.
Extent of Generalization	• Need to generalize across base-models, and *ideally*, across tasks.
Parameterization Challenges	• Need to parameterize the space of base-models – unclear how we can do this.
Examples	• Hyperparameter optimization – does not generalize across tasks • (Bradzil et al., 2003), (Schmidhuber, 2004), (Hochreiter et al., 2001)

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Learning *Which Model* to Learn

- (Bradzil et al., 2003): Enumerate a small set of base-models – not expressive.
- (Schmidhuber, 2004): Search over the space of all possible programs – takes exponential time.
- (Hochreiter et al., 2001): Search over base-models represented by a single step of a recurrent neural net – not expressive.
- Hyperparameter optimization: Search over a predefined set of hyperprameters – not expressive.

Goal	• Learn which base-model is best suited for a task.
Meta-knowledge	• Correlations between different base-models and their performance on different tasks.
Extent of Generalization	• Need to generalize across base-models, and *ideally*, across tasks.
Parameterization Challenges	• Need to parameterize the space of base-models – unclear how we can do this.
Examples	• Hyperparameter optimization – does not generalize across tasks • (Bradzil et al., 2003), (Schmidhuber, 2004), (Hochreiter et al., 2001)

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Learning *How* to Learn

Goal	• Learn how to train the base-model. • Learn about the *process*, rather the *outcome* of learning.
Meta-knowledge	• Commonalities in the behaviours of learning algorithms that achieve good performance.
Extent of Generalization	• Need to generalize across *dissimilar* tasks and/or *similar* base-models.
Parameterization Challenges	• Need to parameterize the space of learning algorithms. • Key Idea: Parameterize the update formula in optimizer.
Examples	• (Bengio et al., 1991) – learned algorithm indep. of tasks/base-models • (Li & Malik, 2016), (Andrychowicz et al., 2016), etc.

For More Details…

Learning to Optimize

Ke Li, Jitendra Malik

arXiv:1606.01885, 2016 and *ICLR*, 2017

Learning to Optimize Neural Nets

Ke Li, Jitendra Malik

arXiv:1703.00441, 2017

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