Advanced Meta-Learning 2:
Large-Scale Meta-Optimization

CS 330

Reminder

HW3 out this Monday, due **next Wednesday.**

Do meta-learning methods scale?

Hand-designed priors

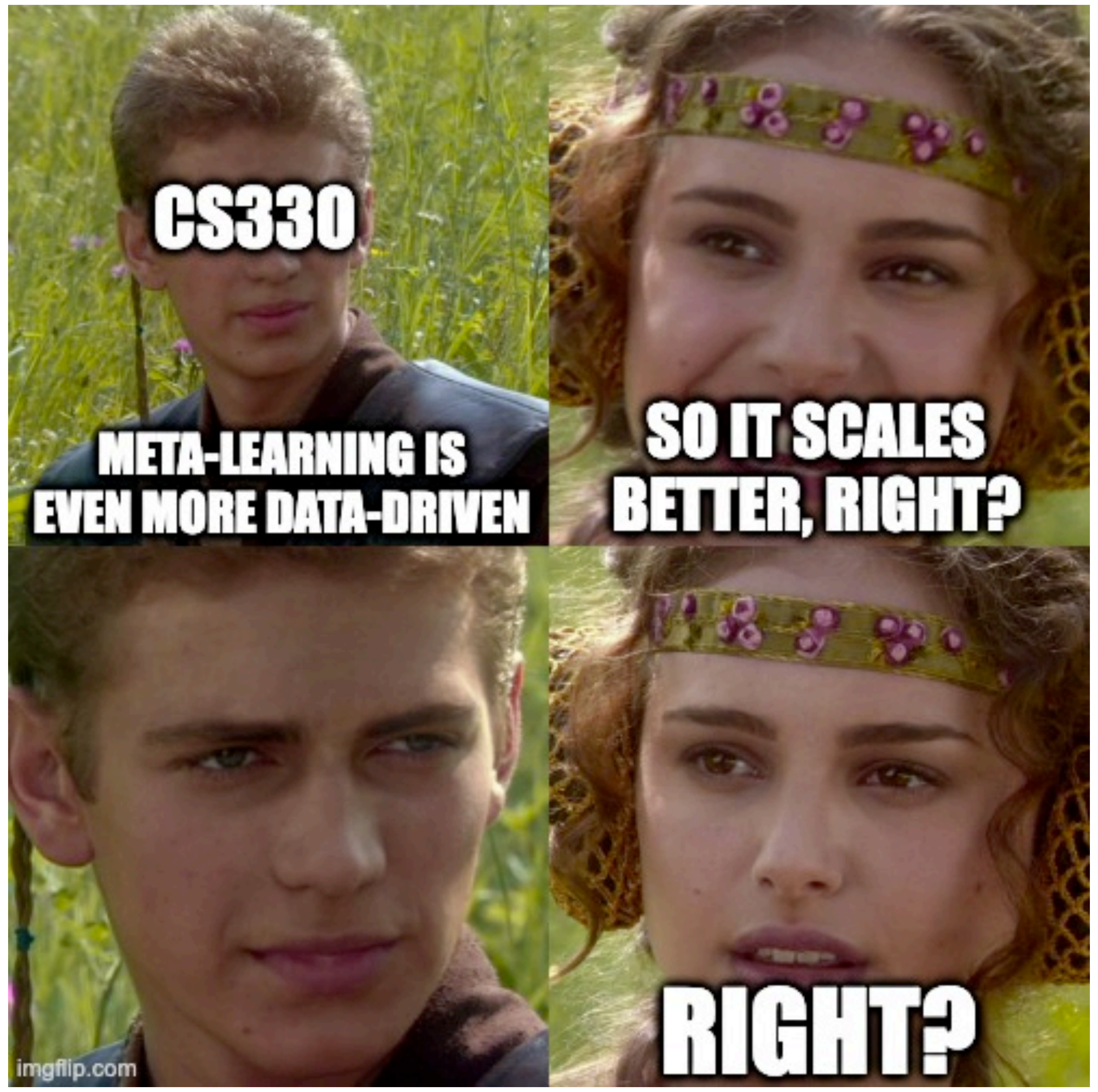
Data-driven priors

Modeling image formation

SIFT features

Fine-tuning from ImageNet

Meta-learning



More data-driven approaches are supposed to be more scalable

Do meta-learning methods work at scale?

Plan for Today

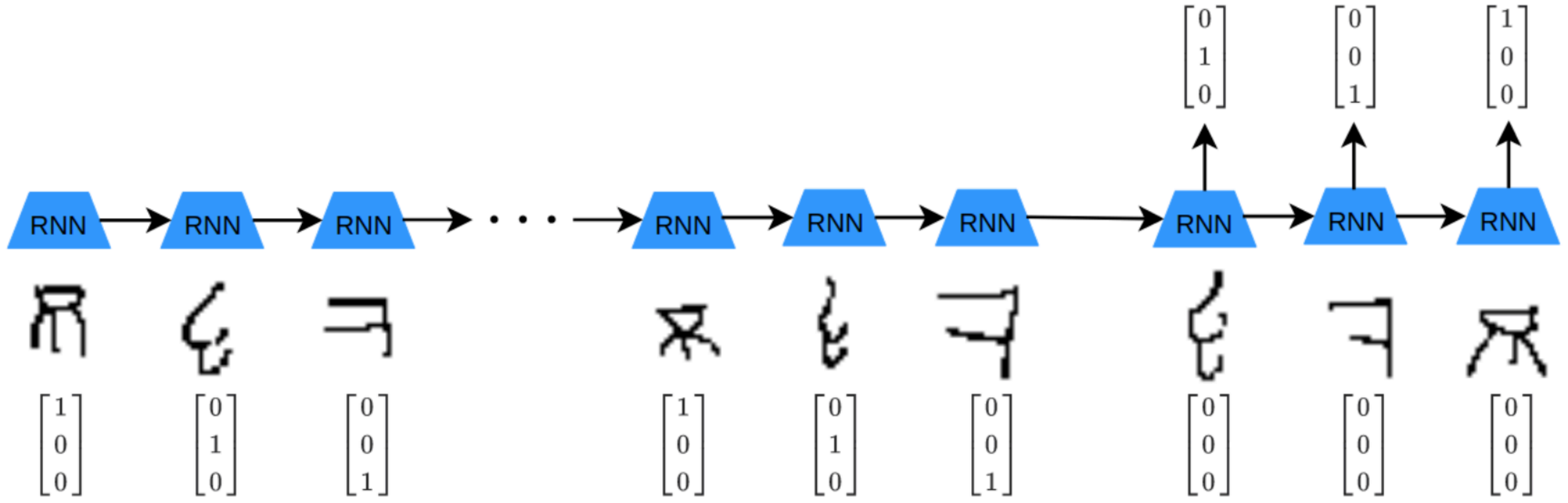
Why consider ***large-scale meta-optimization***?

Applications

Approaches
- Truncated backpropagation
- Gradient-free optimization

Goals for by the end of lecture:
- Know scenarios where existing meta-learning approaches fail due to scale
- Understand techniques for large-scale meta-optimization

Direct Backpropagation

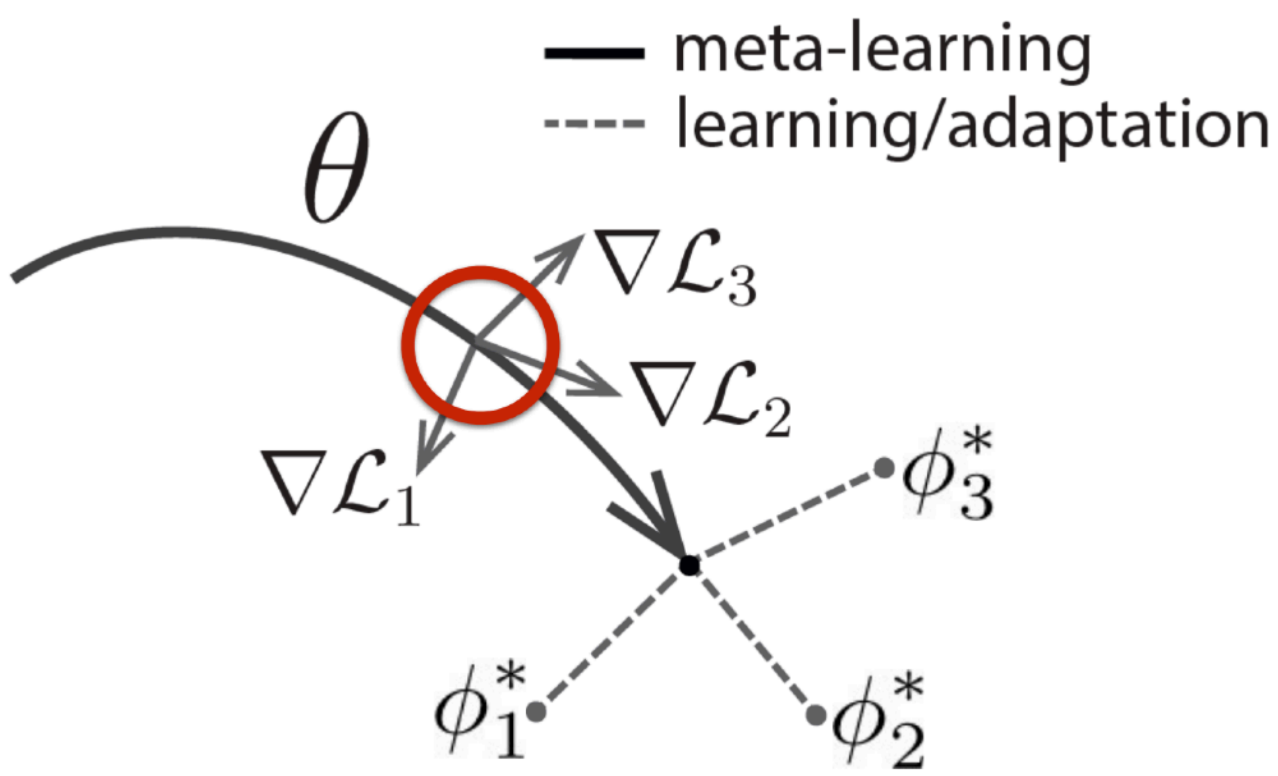


Black-box

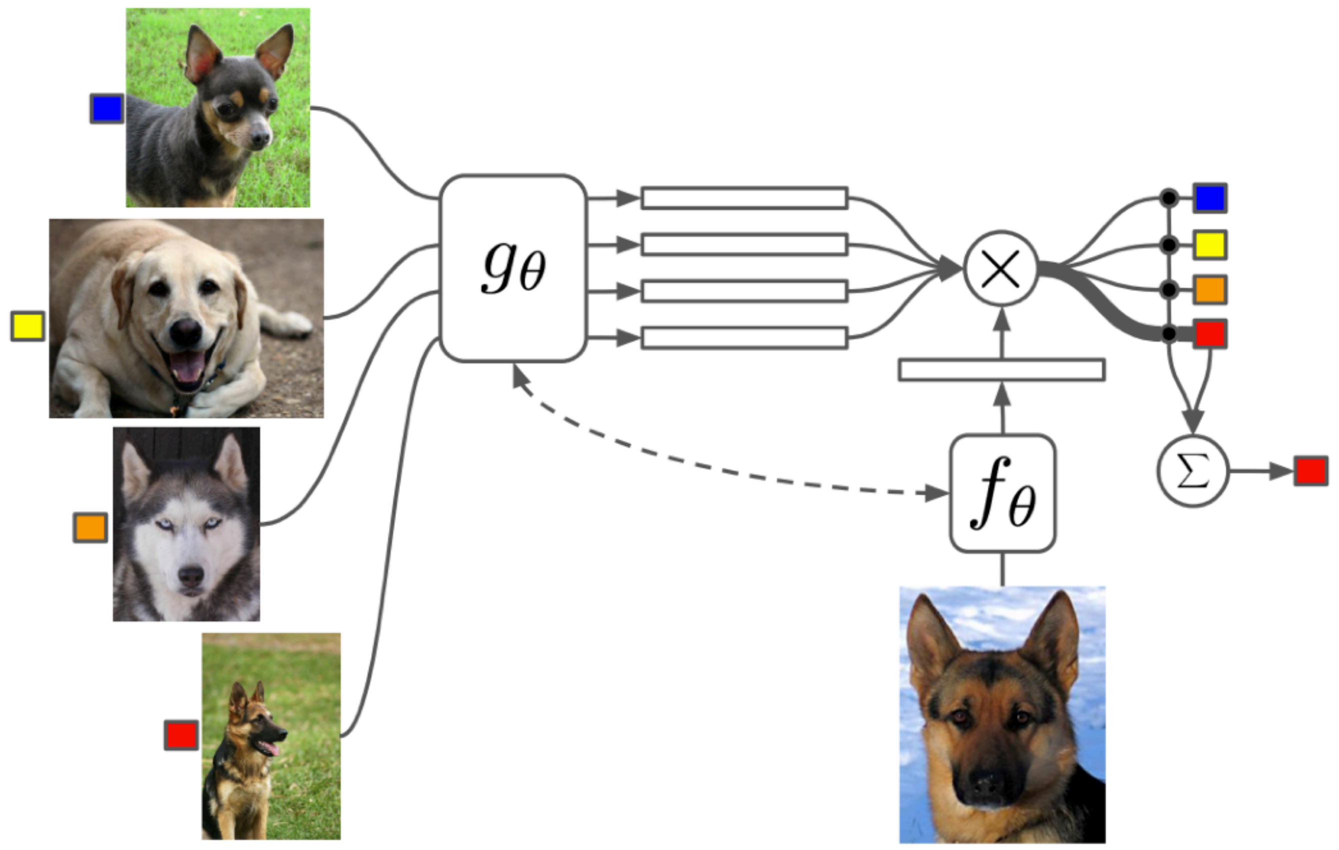
General recipe: Build an inner computation graph, then backpropagate.

+ Automatically works with any differentiable computation graph

- **Memory cost** scales with **computation graph size!**



Optimization-based



Nonparametric

How Big are Computation Graphs?

model	backbone	miniImageNet 5-way 1-shot	miniImageNet 5-way 5-shot	tieredImageNet 5-way 1-shot	tieredImageNet 5-way 5-shot
Meta-Learning LSTM* [22]	64-64-64-64	43.44 ± 0.77	60.60 ± 0.71	-	-
Matching Networks* [33]	64-64-64-64	43.56 ± 0.84	55.31 ± 0.73	-	-
MAML [8]	32-32-32-32	48.70 ± 1.84	63.11 ± 0.92	51.67 ± 1.81	70.30 ± 1.75
Prototypical Networks*† [28]	64-64-64-64	49.42 ± 0.78	68.20 ± 0.66	53.31 ± 0.89	72.69 ± 0.74
Relation Networks* [29]	64-96-128-256	50.44 ± 0.82	65.32 ± 0.70	54.48 ± 0.93	71.32 ± 0.78
R2D2 [3]	96-192-384-512	51.2 ± 0.6	68.8 ± 0.1	-	-
Transductive Prop Nets [14]	64-64-64-64	55.51 ± 0.86	69.86 ± 0.65	59.91 ± 0.94	73.30 ± 0.75
SNAIL [18]	ResNet-12	55.71 ± 0.99	68.88 ± 0.92	-	-
Dynamic Few-shot [10]	64-64-128-128	56.20 ± 0.86	73.00 ± 0.64	-	-
AdaResNet [19]	ResNet-12	56.88 ± 0.62	71.94 ± 0.57	-	-
TADAM [20]	ResNet-12	58.50 ± 0.30	76.70 ± 0.30	-	-
Activation to Parameter† [21]	WRN-28-10	59.60 ± 0.41	73.74 ± 0.19	-	-
LEO† [25]	WRN-28-10	61.76 ± 0.08	77.59 ± 0.12	$\mathbf{66.33 \pm 0.05}$	$\mathbf{81.44 \pm 0.09}$
MetaOptNet-RR (ours)	ResNet-12	61.41 ± 0.61	77.88 ± 0.46	$\mathbf{65.36 \pm 0.71}$	$\mathbf{81.34 \pm 0.52}$
MetaOptNet-SVM (ours)	ResNet-12	62.64 ± 0.61	78.63 ± 0.46	$\mathbf{65.99 \pm 0.72}$	$\mathbf{81.56 \pm 0.53}$
MetaOptNet-SVM-trainval (ours)†	ResNet-12	$\mathbf{64.09 \pm 0.62}$	$\mathbf{80.00 \pm 0.45}$	$\mathbf{65.81 \pm 0.74}$	$\mathbf{81.75 \pm 0.53}$

4-layer CNN
Parameters: <1e5

WRN-28-10
Parameters: <4e6

ResNet-12
Parameters: <1e7

From: "Meta-Learning with Differentiable Convex Optimization", Lee et al.

How Big are Computation Graphs?

```python
class NeuralNetwork(nn.Module):
    def __init__(self):
        super().__init__()
        self.flatten = nn.Flatten()
        self.linear_relu_stack = nn.Sequential(
            nn.Linear(28*28, 512),
            nn.ReLU(),
            nn.Linear(512, 512),
            nn.ReLU(),
            nn.Linear(512, 10)
        )

    def forward(self, x):
        x = self.flatten(x)
        logits = self.linear_relu_stack(x)
        return logits
```

```python
epochs = 5
for t in range(epochs):
    print(f"Epoch {t+1}\n-------------------------------")
    train(train_dataloader, model, loss_fn, optimizer)
    test(test_dataloader, model, loss_fn)
print("Done!")
```

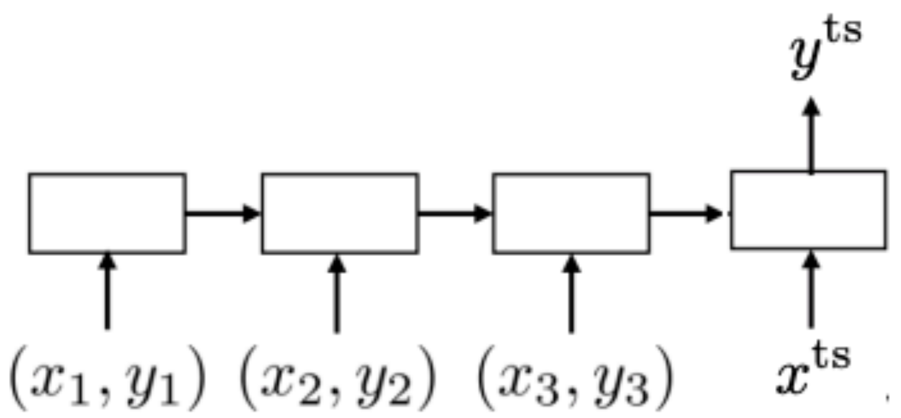
Toy 2-layer MLP from official PyTorch tutorial
Parameters: <7e6
Gradient steps: 5 epochs = ~4e3

Total floats: ~2e10 (>100GB!)

From: https://pytorch.org/tutorials/beginner/basics/quickstart_tutorial.html

Black-box

$$y^{\text{ts}} = f_{\theta}(\mathcal{D}_i^{\text{tr}}, x^{\text{ts}})$$



Optimization-based

$$\begin{aligned} y^{\text{ts}} &= f_{\text{MAML}}(\mathcal{D}_i^{\text{tr}}, x^{\text{ts}}) \\ &= f_{\phi_i}(x^{\text{ts}}) \end{aligned}$$

$$\text{where } \phi_i = \theta - \alpha \nabla_\theta \mathcal{L}(\theta, \mathcal{D}_i^{\text{tr}})$$

Non-parametric

$$\begin{aligned} y^{\text{ts}} &= f_{\text{PN}}(\mathcal{D}_i^{\text{tr}}, x^{\text{ts}}) \\ &= \text{softmax}(-d\left(f_{\theta}(x^{\text{ts}}), \mathbf{c}_n\right)) \end{aligned}$$

$$\text{where } \mathbf{c}_n = \frac{1}{K} \sum_{(x,y) \in \mathcal{D}_i^{\text{tr}}} \mathbb{1}(y = n) f_\theta(x)$$

$$y^{\text{ts}} = f_{\text{LEARN}}\left(\mathcal{D}_i^{\text{tr}}, x^{\text{ts}} \; ; \theta\right)$$

Question: when might f_{LEARN} be too big to apply direct backpropagation?

Settings With Bigger Computation Graphs

$$y^{\text{ts}} = f_{\text{LEARN}}\left(\mathcal{D}_i^{\text{tr}}, x^{\text{ts}} ; \theta\right)$$

Computation graph of f_{LEARN} is large when:

- It uses a big network and/or many gradient steps
- It includes second-order optimization (***meta-meta learning***?)

Meta-parameter θ can be any component of f_{LEARN}:

HW2
- Initial parameters
- Learning rate
- Optimizer
- Loss function
- Dataset
- Network architecture

$$\min_{\theta} \sum_{\text{task}_i} \left(\theta - \alpha \nabla_\theta L\left(\theta, D_i^{\text{tr}}\right), D_i^{\text{ts}}\right)$$

$$\min_{\theta,\alpha} \sum_{\text{task}_i} \left(\theta - \alpha \nabla_\theta L\left(\theta, D_i^{\text{tr}}\right), D_i^{\text{ts}}\right)$$

$$\min_{\theta,\psi} \sum_{\text{task}_i} \left(\theta - \alpha \nabla_\theta L_\psi\left(\theta, D_i^{\text{tr}}\right), D_i^{\text{ts}}\right)$$

$$\min_{\omega} \sum_{\theta \sim p(\theta_0)} \left(\theta - \alpha \nabla_\theta L\left(\theta, D_\omega\right), D_i^{\text{ts}}\right)$$

Plan for Today

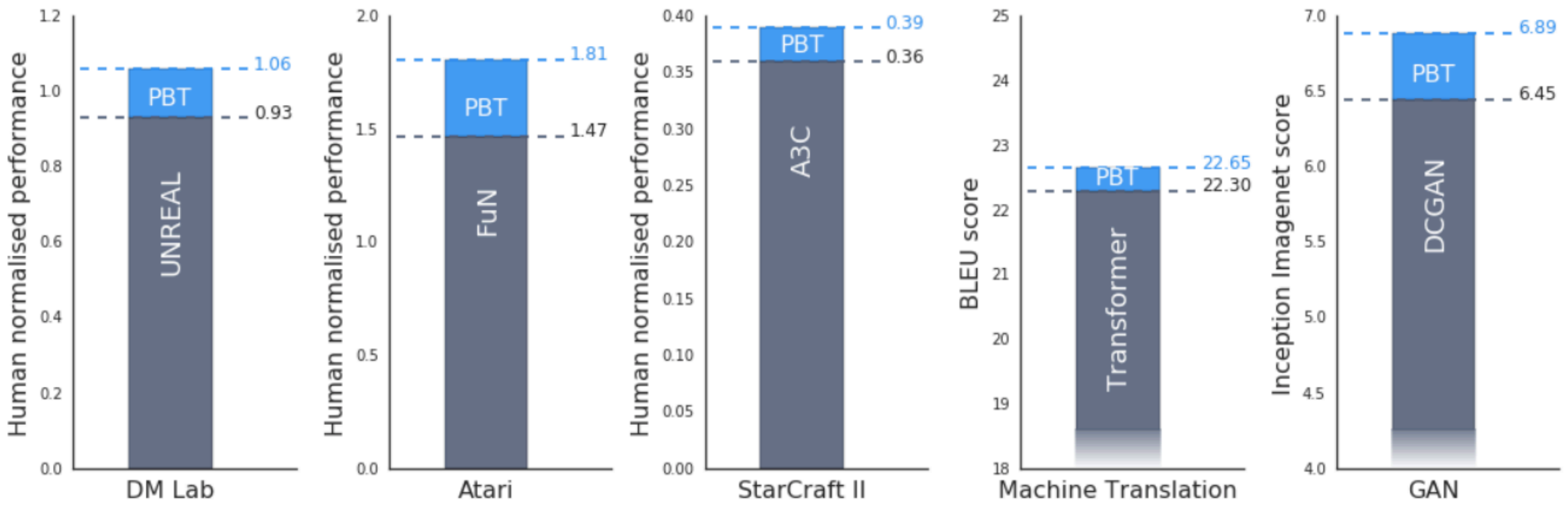
Why consider large-scale meta-optimization?

Applications

Approaches
- Truncated backpropagation
- Gradient-free optimization

Application: Hyperparameter Optimization

Goal: Optimize ***hyperparameters*** for validation set performance



Benefits over random search in many domains

Method	Validation	Test	Time(s)
Grid Search	97.32	94.58	100k
Random Search	84.81	81.46	100k
Bayesian Opt.	72.13	69.29	100k
STN	70.30	67.68	25k
No HO	75.72	71.91	18.5k
Ours	69.22	66.40	18.5k
Ours, Many	**68.18**	**66.14**	18.5k

LSTM Hyperparameters

Inverse Approx.	Validation	Test
0	92.5 ±0.021	92.6 ±0.017
3 Neumann	**95.1** ±0.002	94.6 ±0.001
3 Unrolled Diff.	95.0 ±0.002	**94.7** ±0.001
I	94.6 ±0.002	94.1 ±0.002

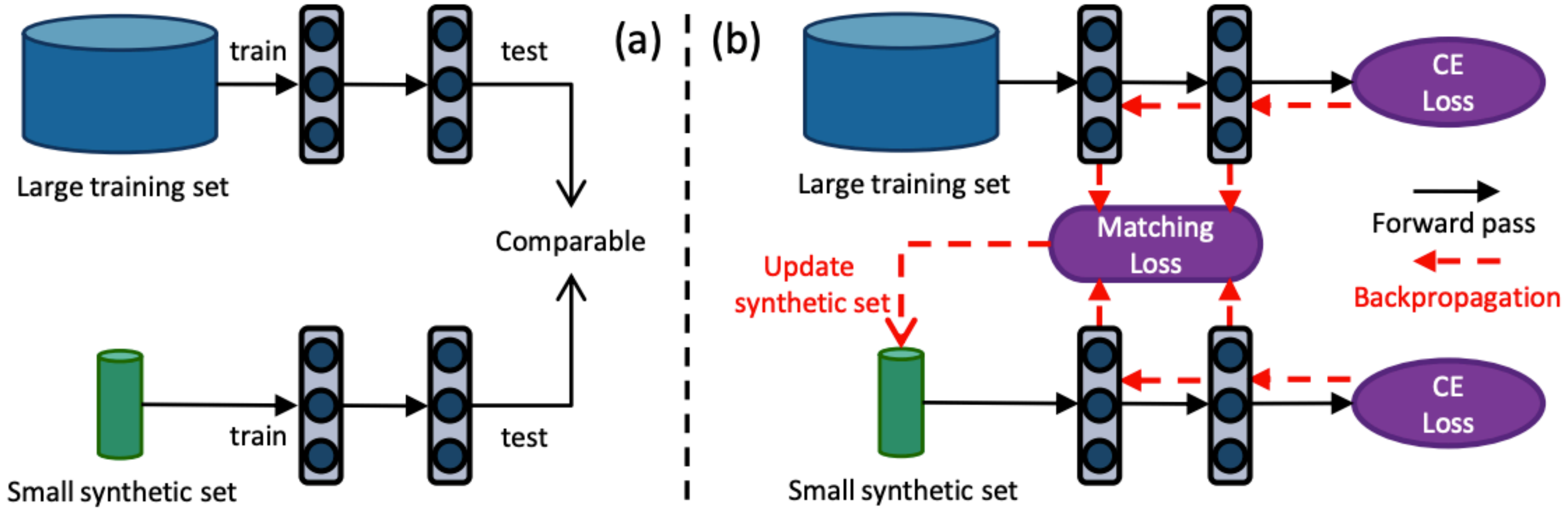
“Hyper”parameters of a data augmentation network

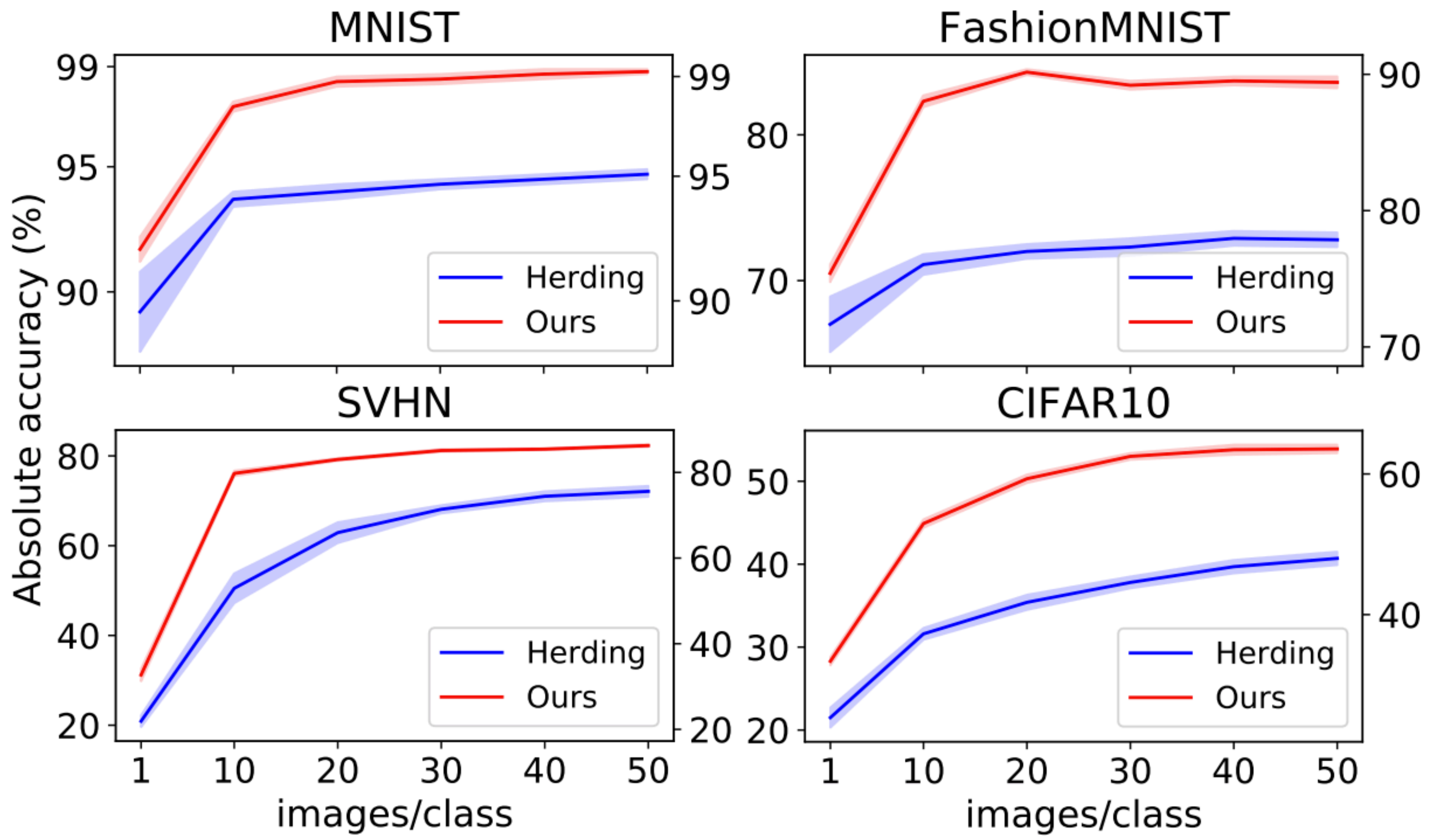
From: “Population Based Training of Neural Networks”, Jaderberg et al. (2017)

From: “Optimizing Millions of Hyperparameters by Implicit Differentiation”, Lorraine et al. (2019)

Application: Dataset Distillation

Goal: optimize a ***synthetic training set*** for validation set performance



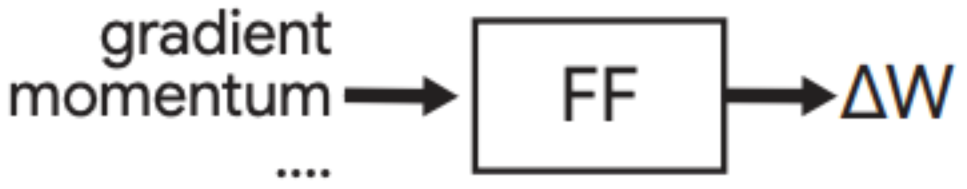


Method: Match training data gradients at each timestep

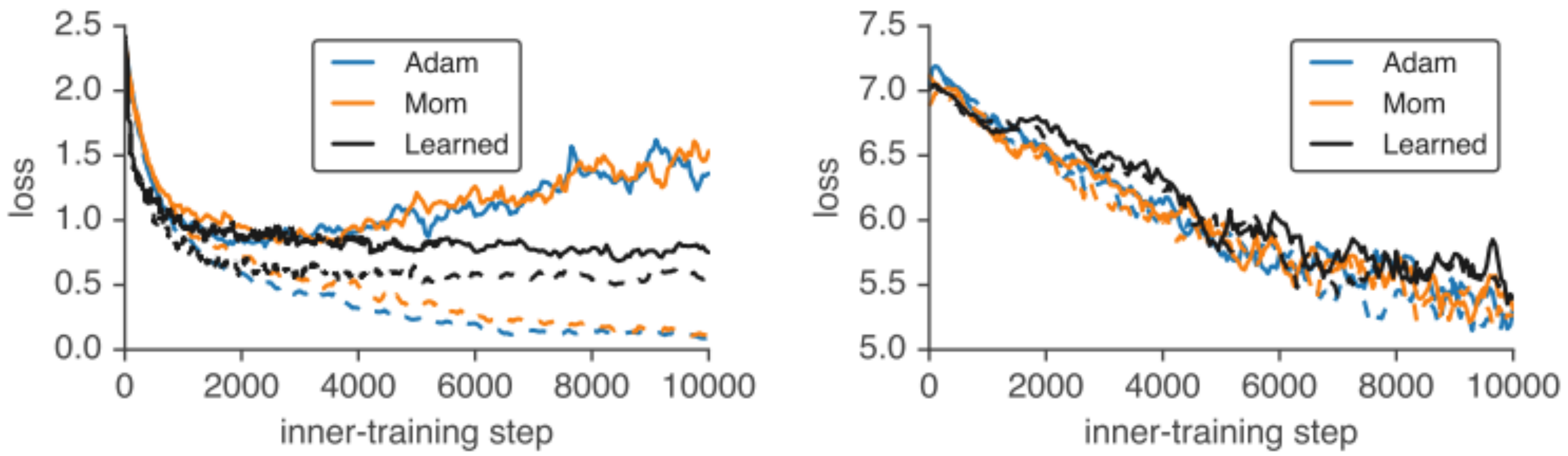
From: "Dataset Condensation with Gradient Matching", Zhao et al. (2020)

Application: Optimizer Learning

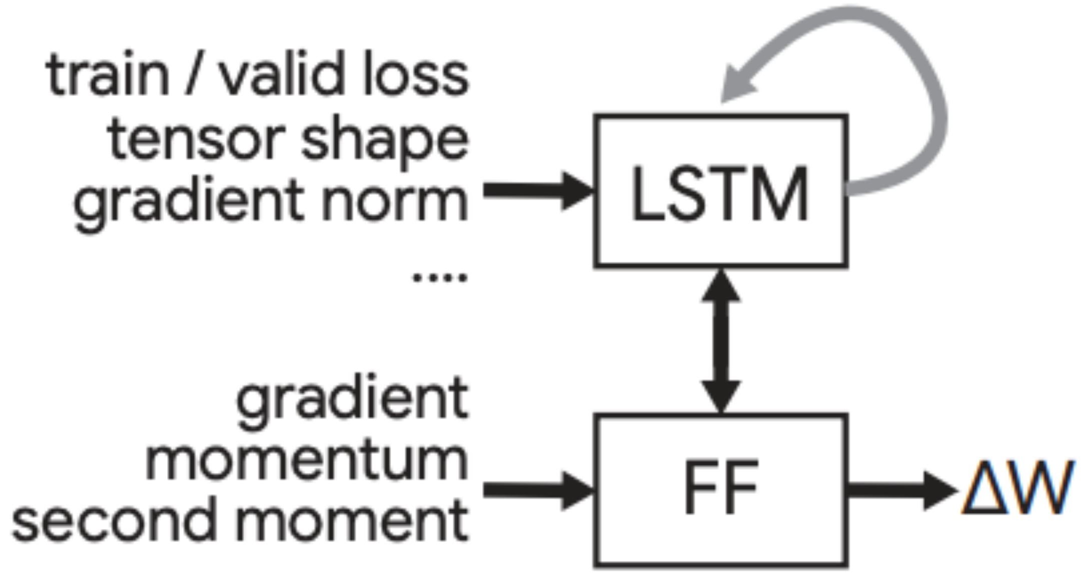
Goal: Optimize an ***optimizer*** for validation set performance



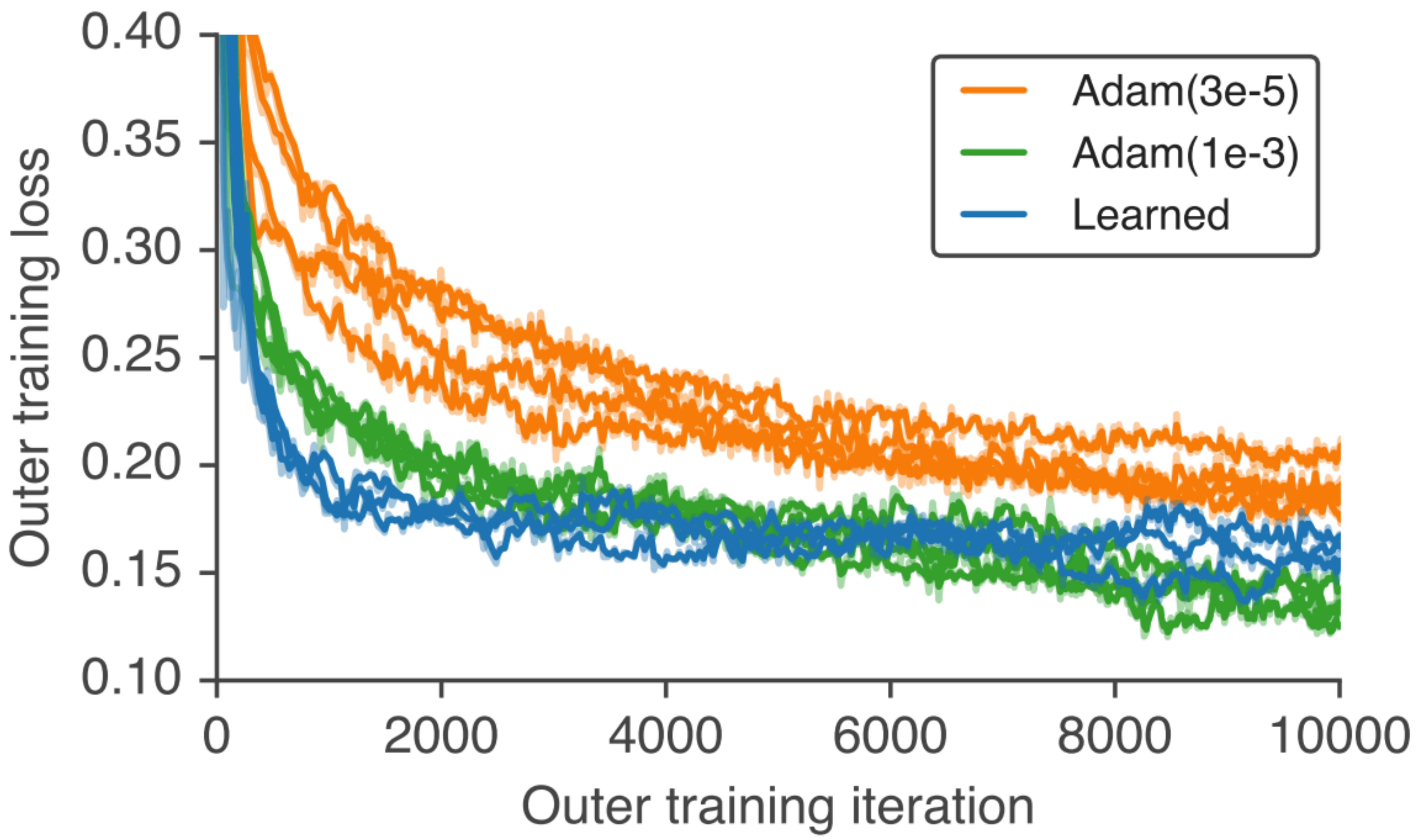
Simple architecture



Works at ResNet scale



More complex architecture
with per-tensor LSTM

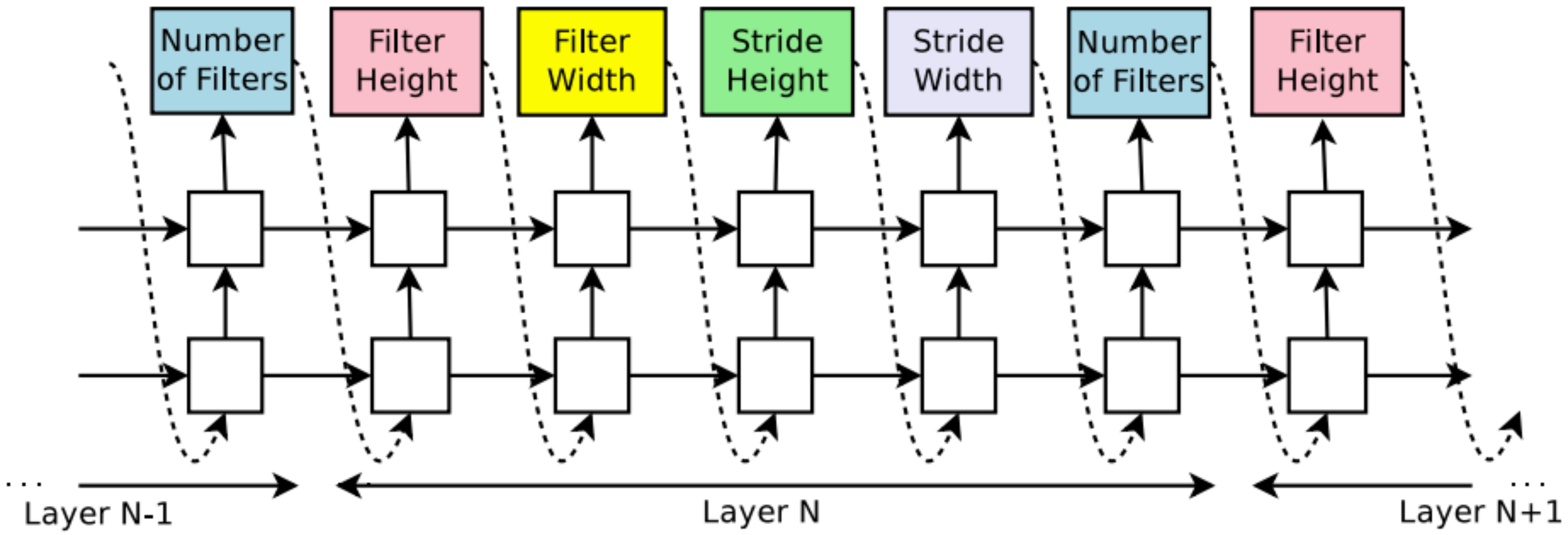


Can even train itself

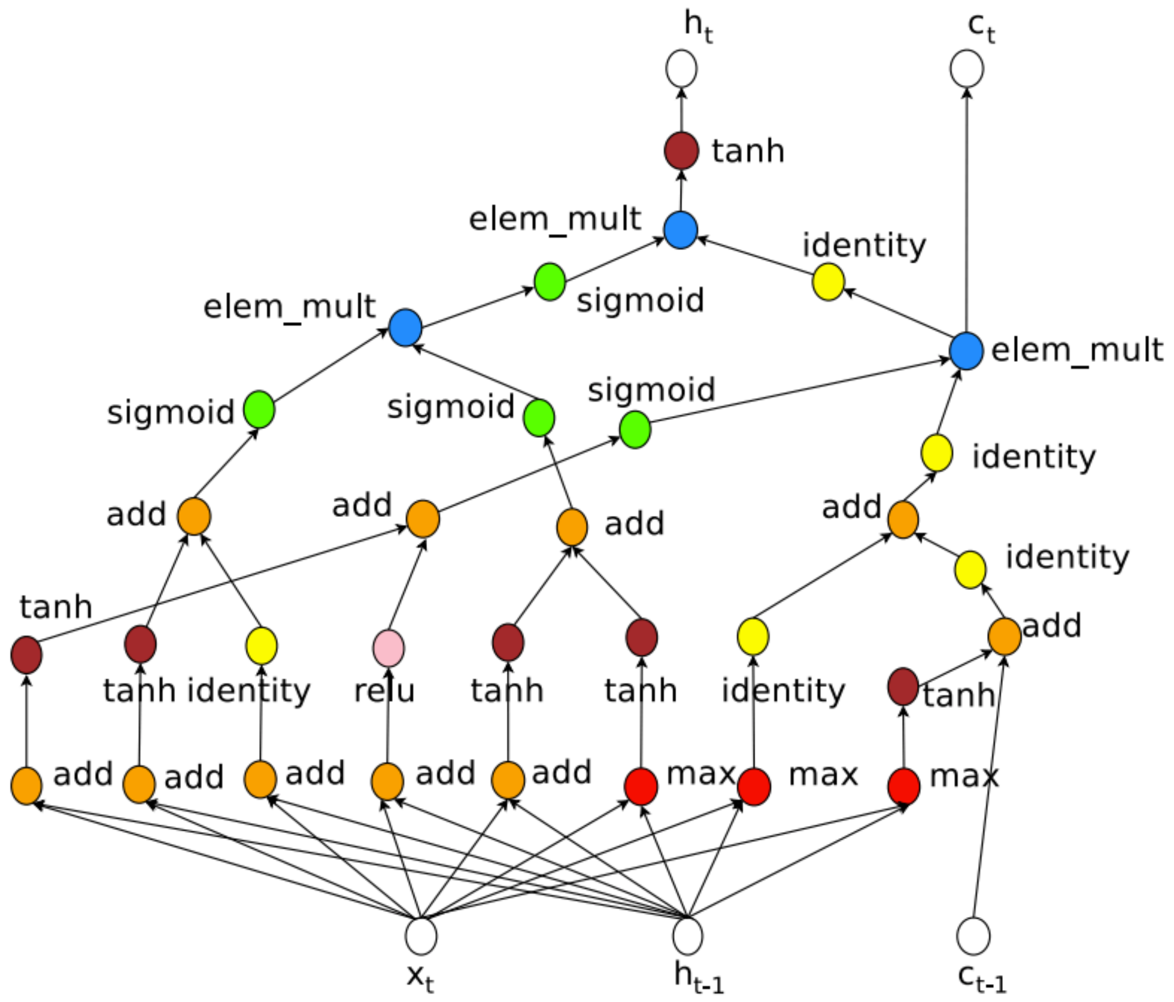
From: "Tasks, stability, architecture, and compute: Training more effective learned optimizers, and using them to train themselves", Metz et al. (2020)

Application: Neural Architecture Search

Goal: Optimize an ***architecture*** for validation set performance



An RNN parameterizes a neural network



A generated cell for an RNN

Model	Depth	Parameters	Error rate (%)
Network in Network (Lin et al., 2013)	-	-	8.81
All-CNN (Springenberg et al., 2014)	-	-	7.25
Deeply Supervised Net (Lee et al., 2015)	-	-	7.97
Highway Network (Srivastava et al., 2015)	-	-	7.72
Scalable Bayesian Optimization (Snoek et al., 2015)	-	-	6.37
FractalNet (Larsson et al., 2016)	21	38.6M	5.22
with Dropout/Drop-path	21	38.6M	4.60
ResNet (He et al., 2016a)	110	1.7M	6.61
ResNet (reported by Huang et al. (2016c))	110	1.7M	6.41
ResNet with Stochastic Depth (Huang et al., 2016c)	110	1.7M	5.23
	1202	10.2M	4.91
Wide ResNet (Zagoruyko & Komodakis, 2016)	16	11.0M	4.81
	28	36.5M	4.17
ResNet (pre-activation) (He et al., 2016b)	164	1.7M	5.46
	1001	10.2M	4.62
DenseNet ($L = 40, k = 12$) Huang et al. (2016a)	40	1.0M	5.24
DenseNet($L = 100, k = 12$) Huang et al. (2016a)	100	7.0M	4.10
DenseNet ($L = 100, k = 24$) Huang et al. (2016a)	100	27.2M	3.74
DenseNet-BC ($L = 100, k = 40$) Huang et al. (2016b)	190	25.6M	3.46
Neural Architecture Search v1 no stride or pooling	15	4.2M	5.50
Neural Architecture Search v2 predicting strides	20	2.5M	6.01
Neural Architecture Search v3 max pooling	39	7.1M	4.47
Neural Architecture Search v3 max pooling + more filters	39	37.4M	3.65

Zoph and Le, "Neural Architecture Search with Reinforcement Learning" (2017)

Plan for Today

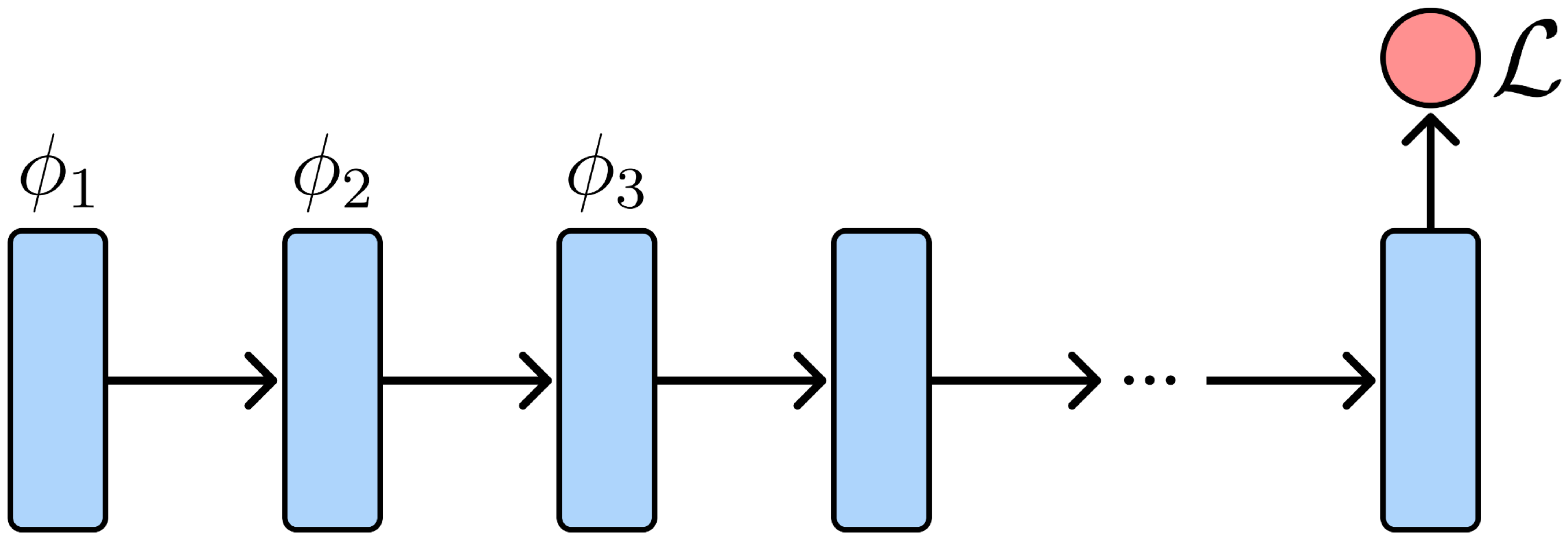
Why consider large-scale meta-optimization?

Applications

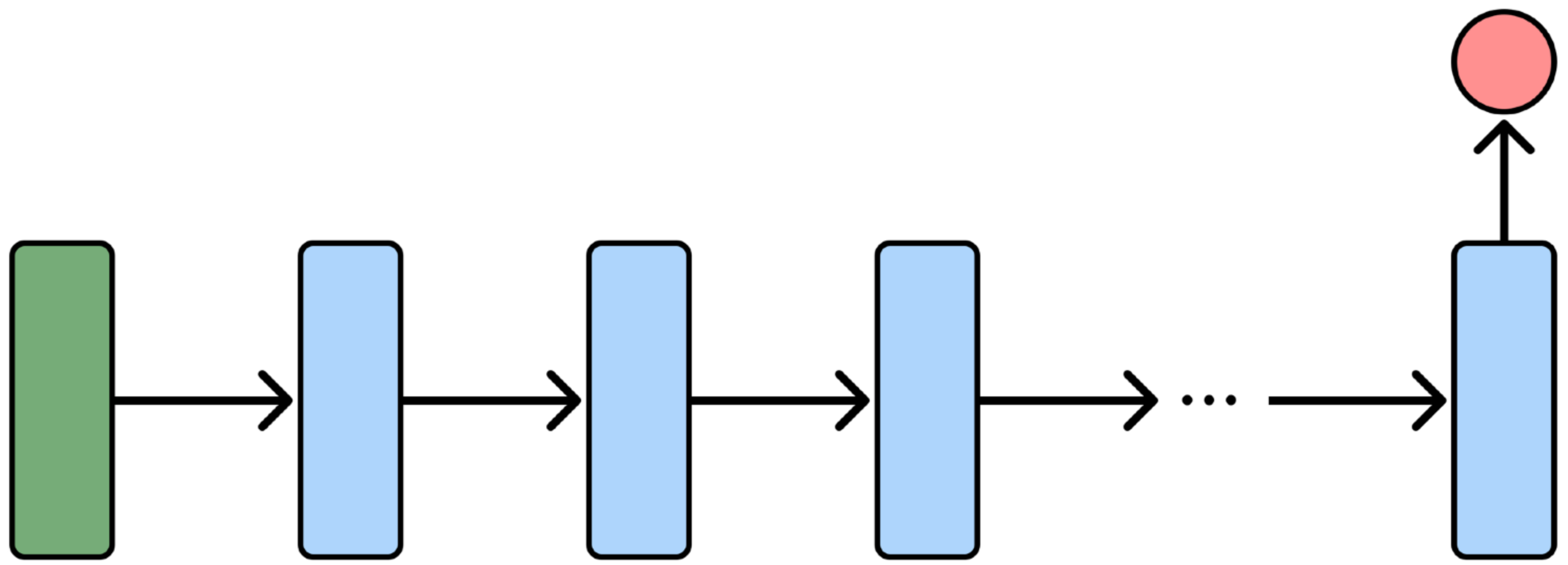
Approaches

- Truncated backpropagation
- Gradient-free optimization

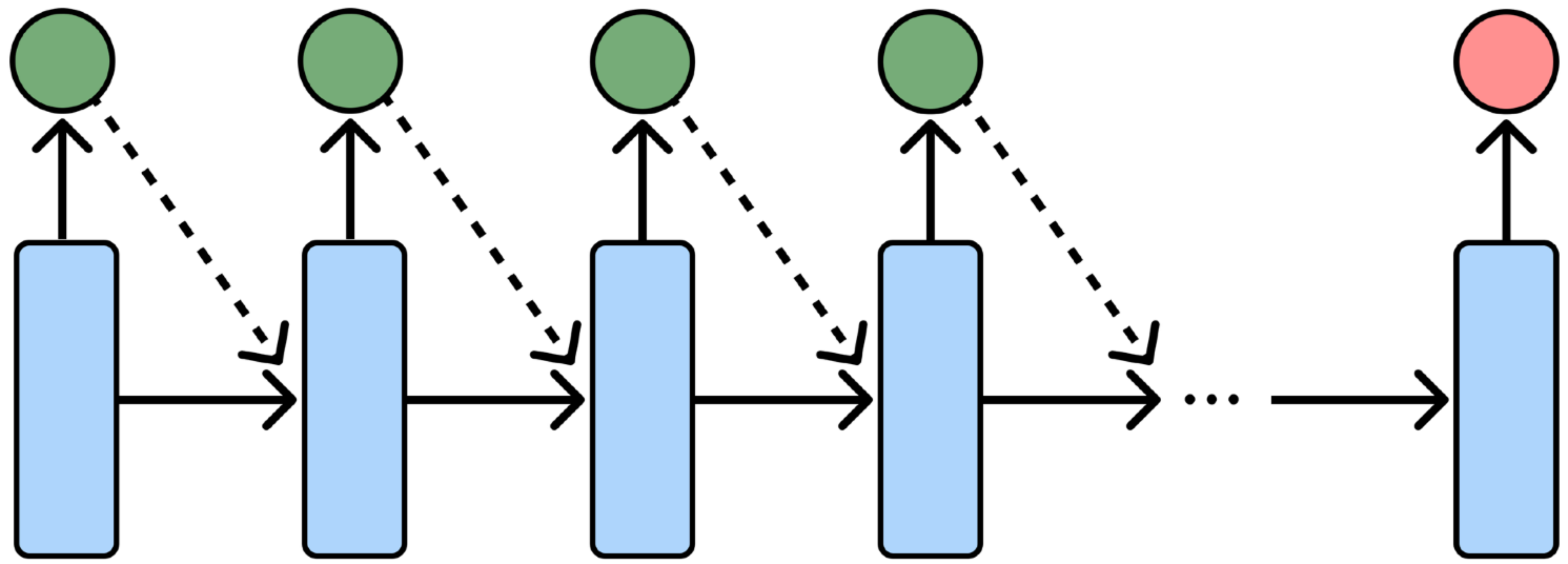
Unrolled Computation Graphs



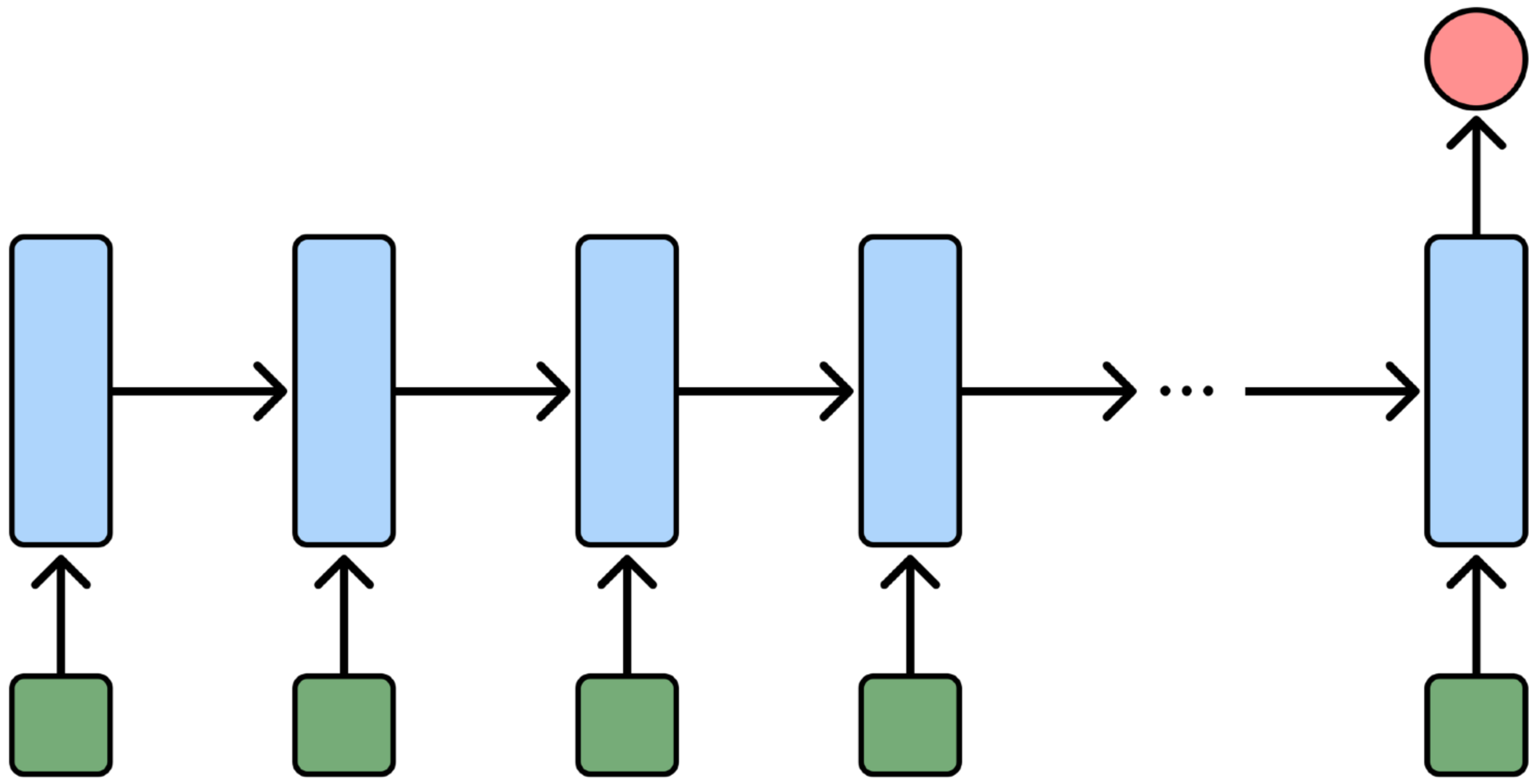
Unrolled Computation Graphs



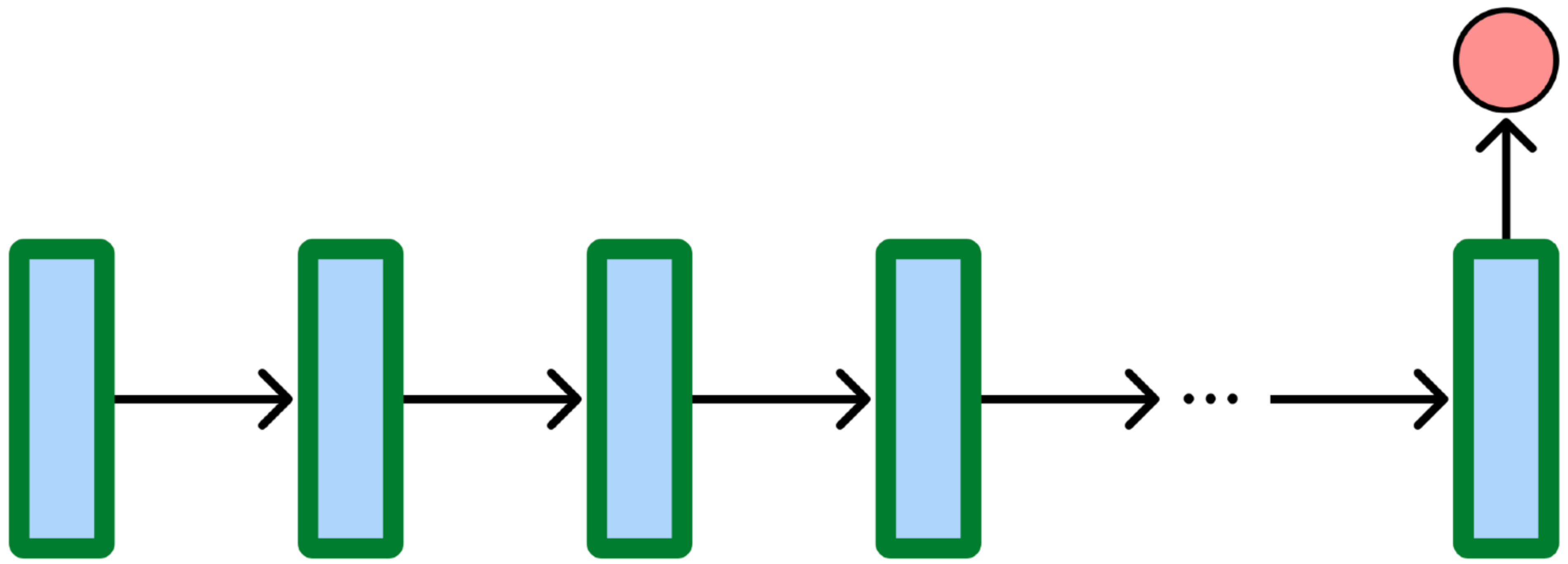
Initial Parameters



Learned loss / Regularizer, Optimizer



Synthetic dataset / augmentation



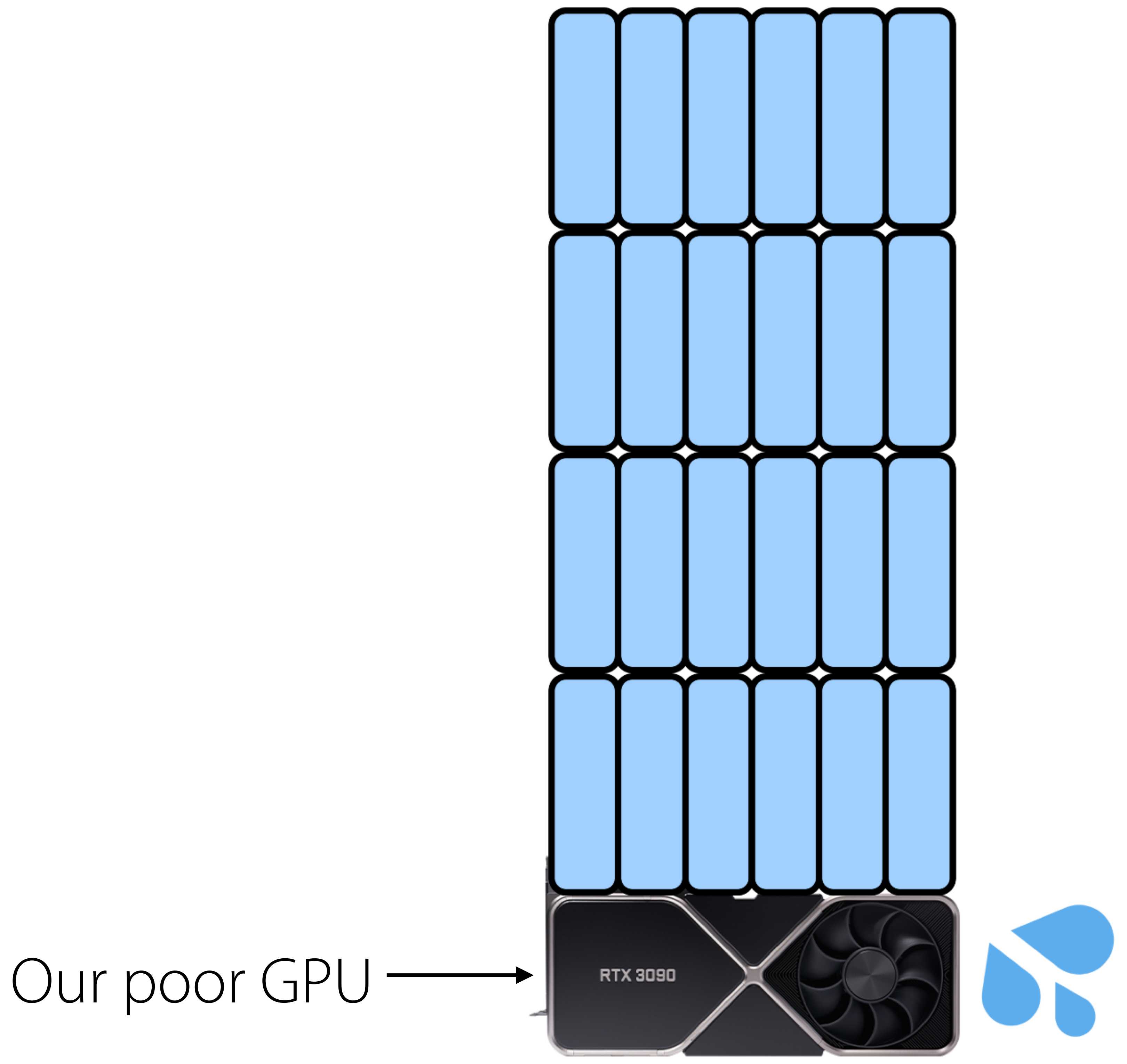
Architecture

Plan for Today

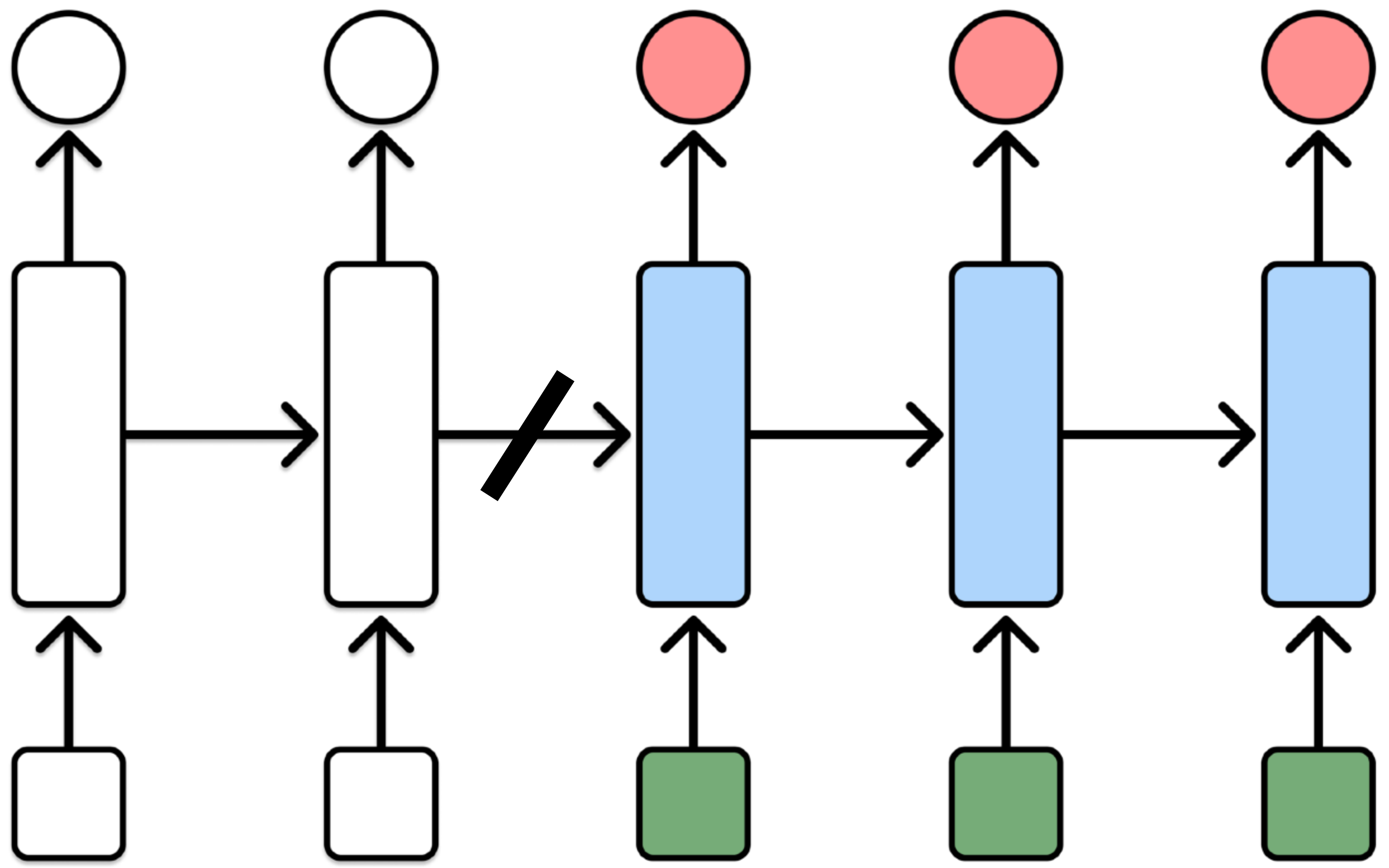
Why consider large-scale meta-optimization?

Applications

Approaches
- **Truncated backpropagation**
- Gradient-free optimization



Truncated Backpropagation



T=3

```
losses = []
for x, y in train_loader:
    y_pred, state = rnn(state)
    losses.append(loss_fn(y, y_pred))
    if len(losses) == T:
        torch.sum(losses).backward()
        opt.step()
        opt.zero_grad()
        state.detach_()
        losses = []
```

Split the full sequence into shorter slices, and backpropagate after processing each slice.

Question: what could happen if we use short T?

\+ **Simple**: autograd handles everything
\- **Biased** estimator
\- Cannot take **long-range dependencies** into account
\- Sequence length introduces a **tradeoff between correctness and memory cost**

Plan for Today

Why consider large-scale meta-optimization?

Applications

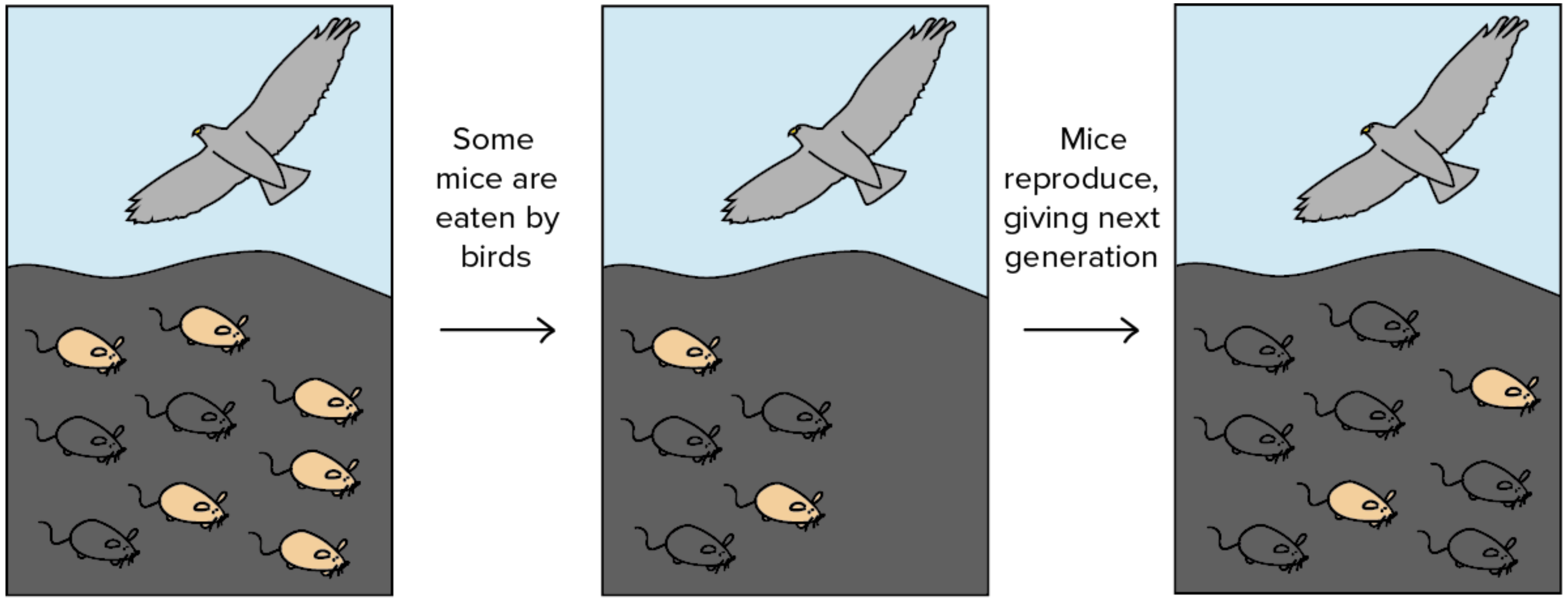
Approaches
- Truncated backpropagation
- **Gradient-free optimization**

Gradient-free Optimization

Backpropagation is costly for large computation graphs…

Optimization **does not necessarily require gradients!**

Evolution Strategies: Estimates gradients using stochastic finite differences.

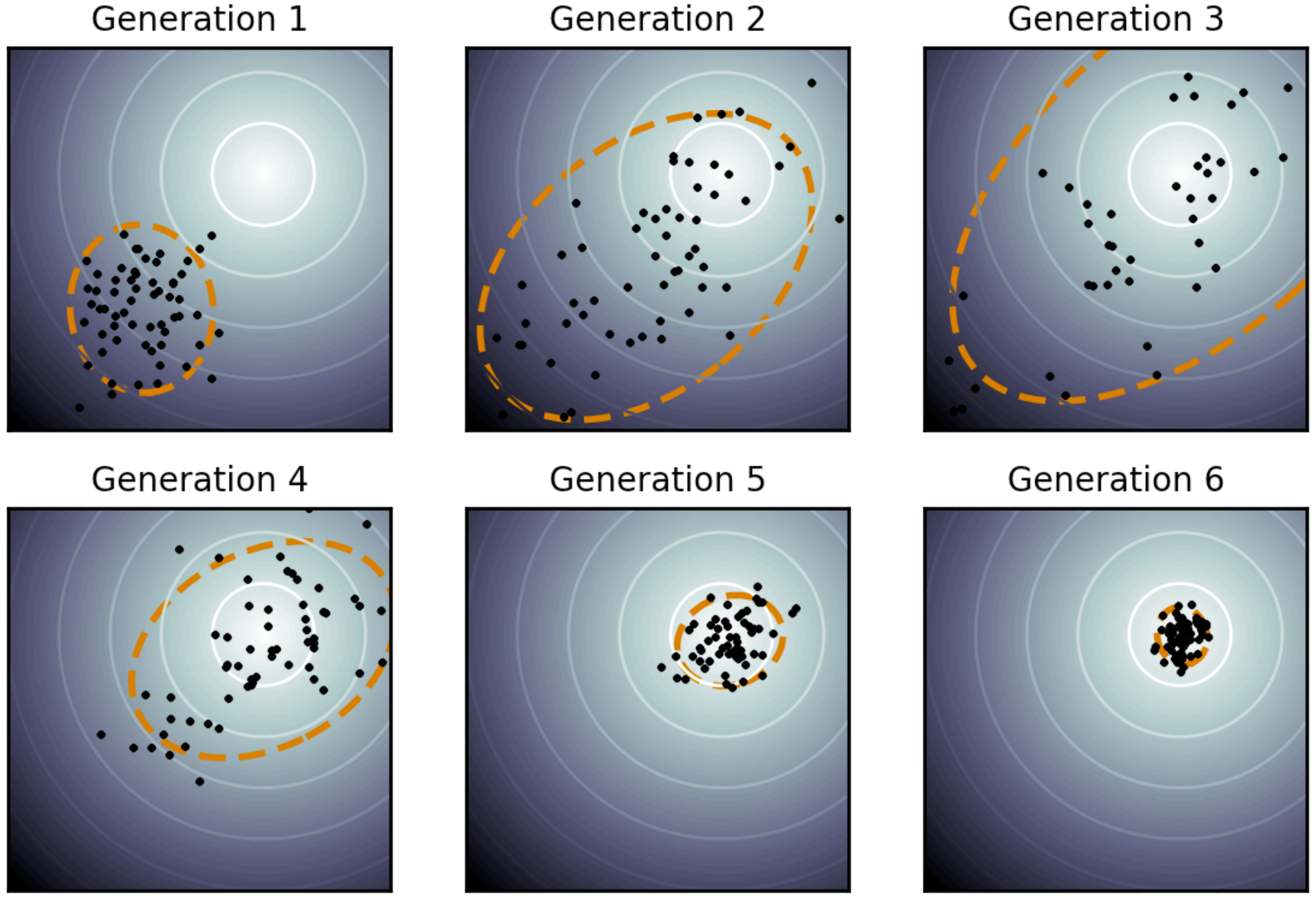


From: Khan Academy: Darwin, evolution, & natural selection

Evolution Strategies

Initialize parameters $(\mu, \sigma) \leftarrow (\mu_0, \sigma_0)$. Repeat:

1. Sample particles: $x^1, x^2, \ldots, x^N \sim \mathcal{N}(\mu, \sigma^2 I)$
2. Evaluate and get best: $\{e^1, \ldots, e^n\} \subset \{x^1, \ldots, x^N\}$
3. $\mu, \sigma^2 \leftarrow \text{Avg}(e^1, \ldots, e^n), \text{Var}(e^1, \ldots, e^n)$



From: Wikipedia CMA-ES page

Example: optimizing **learning rate**

Initialize lr and noise $(\alpha, \sigma) \leftarrow (\alpha_0, \sigma_0)$

1. Sample lr: $\alpha^1, \alpha^2, \ldots, \alpha^N \sim \mathcal{N}(\alpha, \sigma^2)$
2. Run SGD, get runs with best val accuracy: $\{e^1, \ldots, e^n\} \subset \{\alpha^1, \ldots, \alpha^N\}$
3. $\alpha, \sigma^2 \leftarrow \text{Avg}(e^1, \ldots, e^n), \text{Var}(e^1, \ldots, e^n)$

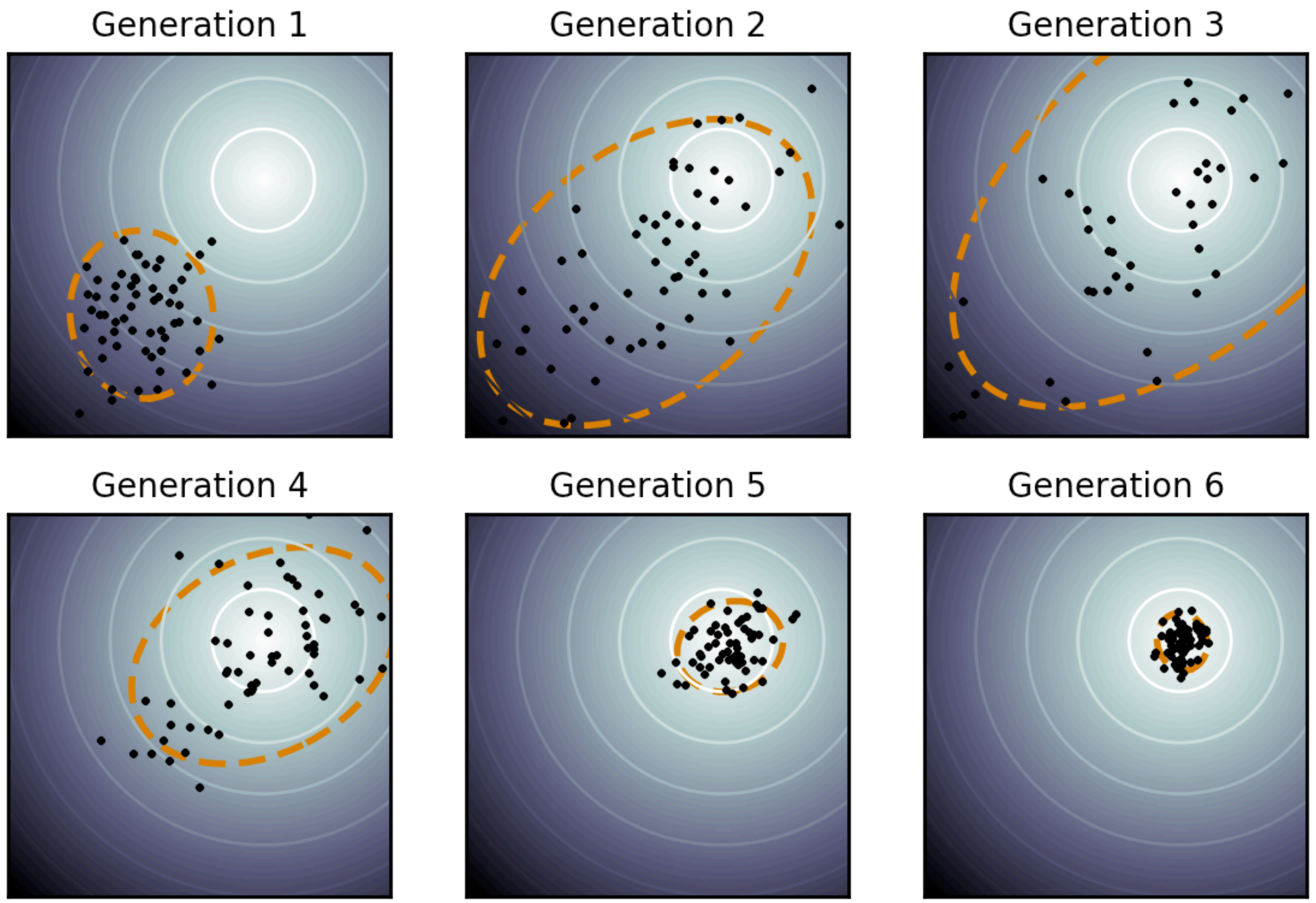
Question: what could happen if we try to optimize **initial parameters** with ES?

Unlikely to observe good initial parameters, because parameter space is high-dimensional.

Evolution Strategies

Initialize parameters $(\mu, \sigma) \leftarrow (\mu_0, \sigma_0)$. Repeat:

1. Sample particles: $x^1, x^2, \ldots, x^N \sim \mathcal{N}(\mu, \sigma^2 I)$
2. Evaluate and get best: $\{e^1, \ldots, e^n\} \subset \{x^1, \ldots, x^N\}$
3. $\mu, \sigma^2 \leftarrow \mathrm{Avg}(e^1, \ldots, e^n), \mathrm{Var}(e^1, \ldots, e^n)$



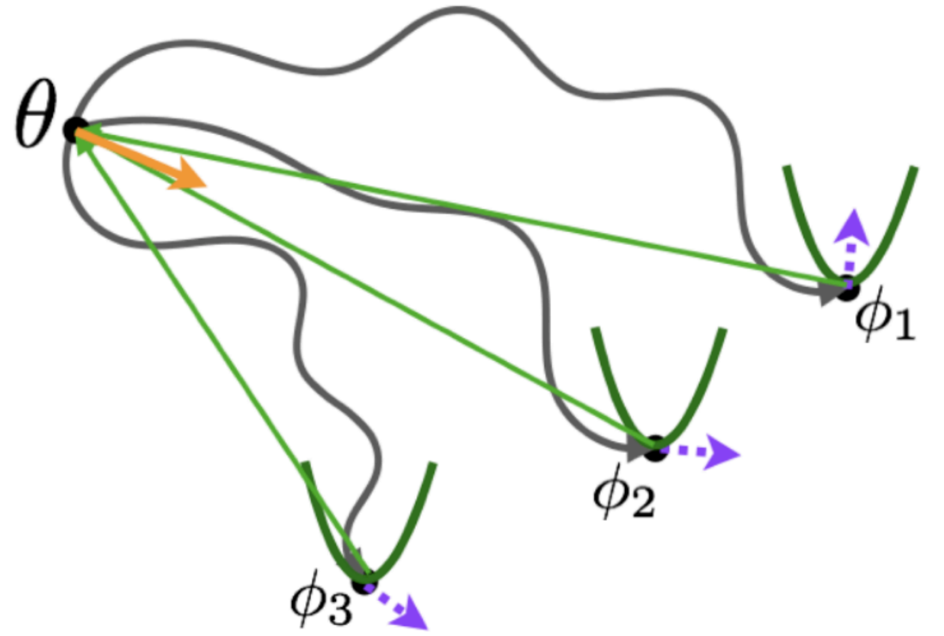
From: Wikipedia CMA-ES page

+ **Constant memory cost**
+ **Parallelizable** across particles
+ Inner steps can be non-differentiable

\- Struggles with **high-dimensional covariates** and/or **complex loss surfaces**

Other Approaches

Implicit Differentiation



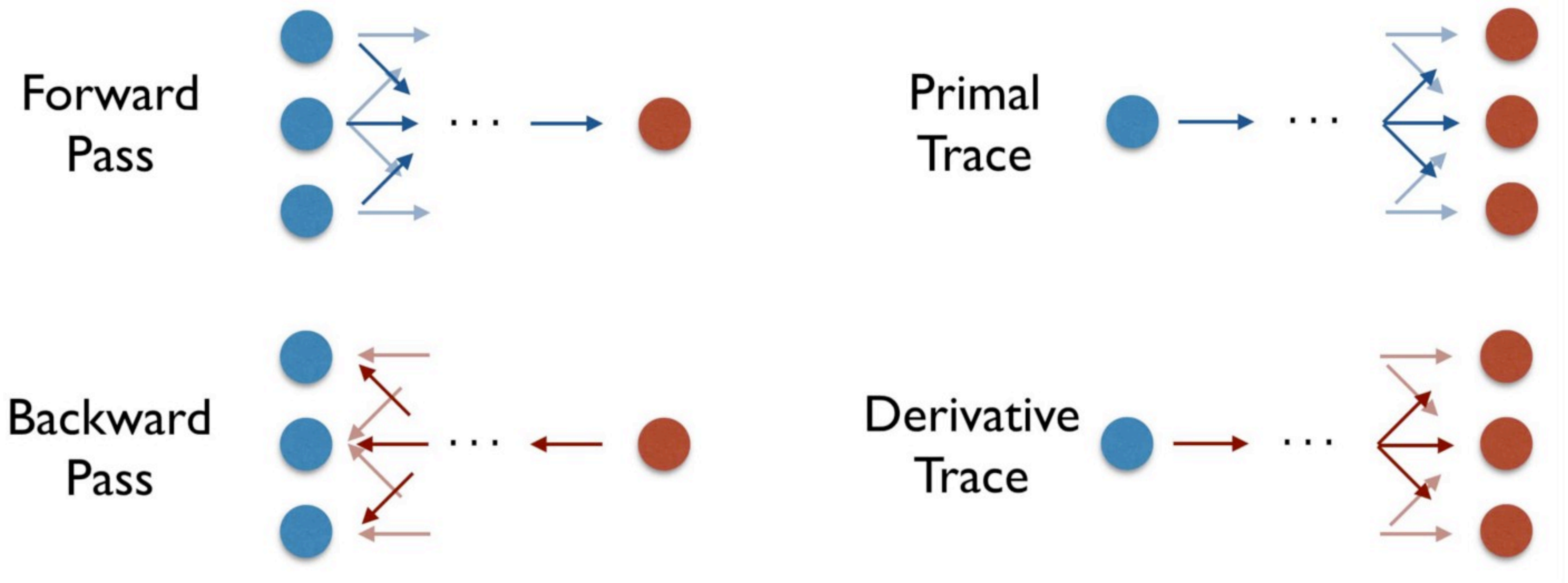
Computes full meta-gradient based only on the final result of the inner loop.

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \, \frac{1}{M} \sum_{i=1}^{M} \boxed{\frac{d\mathcal{A}lg_i^\star(\boldsymbol{\theta})}{d\boldsymbol{\theta}}} \, \nabla_\phi \mathcal{L}_i(\mathcal{A}lg_i^\star(\boldsymbol{\theta})).$$

$$\boxed{\frac{d\mathcal{A}lg_i^\star(\boldsymbol{\theta})}{d\boldsymbol{\theta}}} = \left(\boldsymbol{I} + \frac{1}{\lambda} \nabla_{\boldsymbol{\phi}}^2 \hat{\mathcal{L}}_i(\boldsymbol{\phi}_i) \right)^{-1}$$

From: "Meta-Learning with Implicit Gradients", Rajeswaran et al. (2019)

Forward-mode Differentiation



Uses the chain rule in the opposite direction from backprop, accumulating derivatives from start to finish.

From: "Forward Mode Automatic Differentiation & Dual Numbers", Lange

Plan for Today

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Applications

Approaches
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- Gradient-free optimization

Goals for by the end of lecture:
- Know scenarios where existing meta-learning approaches fail due to scale
- Understand techniques for large-scale meta-optimization