

Adaptation and Universality in First Order Optimization

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Joint work with

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One formula to rule all machine learning problems

$$f^* = \min_{x:x \in \mathcal{X}} f(x) \quad (\text{argmin} \rightarrow x^*)$$

- Growing interest in first-order gradient methods¹ due to their scalability and generalization performance

¹Lan, Guanghui. First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

One formula to rule ~~all~~^{some} machine learning problems ...and one algorithm to solve them.

$$f^* = \min_{x: x \in \mathcal{X}} f(x) \quad (\text{argmin} \rightarrow x^*)$$

- Growing interest in first-order gradient methods¹ due to their scalability and generalization performance
- In the sequel,
 - ▶ the set $\mathcal{X}$ is convex and has a tractable projection operator $P_{\mathcal{X}}$
 - ▶ all convergence characterizations are with feasible iterates $x^k \in \mathcal{X}$
 - ▶ gradient mapping means $G_{\eta}(x^k) = \frac{1}{\eta}[x^k - P_{\mathcal{X}}(x^k - \eta \nabla f(x^k))]$, where η is the step-size
 - ▶ L -smooth means $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|, \forall x, y \in \mathcal{X}$
 - ▶ ∂ may refer to the generalized subdifferential, and $\delta_{\mathcal{X}}$ refers to the indicator function for the set $\mathcal{X}$

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Worst-case iteration complexities of classical projected first-order methods¹²

$f(x)$	gradient oracle	L -smooth	Stationarity measure	GD/SGD	Accelerated GD/SGD
Convex	stochastic	yes	$f(x^k) - f^* =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$
Convex	deterministic	yes	$f(x^k) - f^* =$	$\mathcal{O}\left(\frac{1}{k}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$
Convex	stochastic	no	$f(x^k) - f^* =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$
Nonconvex	stochastic	yes	$\ G_\eta(x^k)\ ^2 =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^3$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^3$
Nonconvex	deterministic	yes	$\ G_\eta(x^k)\ ^2 =$	$\mathcal{O}\left(\frac{1}{k}\right)^4$	$\mathcal{O}\left(\frac{1}{k}\right)^4$
Nonconvex	stochastic	no	$\text{dist}(0, \partial(f(x^k) + \delta_{\mathcal{X}}(x^k)))^2 =$	$\mathfrak{?}^{356}$	$\mathfrak{?}^{356}$

- Basic structures, such as smoothness or strong convexity, help, but there are more structures that can be used:
 - max-form, metric subregularity, Polyak-Lojasiewicz, Kurdyka-Lojasiewicz, weak convexity,³ growth cond...

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²Y. Carmon, J.C. Duchi, O. Hinder, and A. Sidford, "Lower bounds for finding stationary points I-II." Mathematical Programming, 2019.

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⁴S. Ghadimi and G. Lan, "Accelerated gradient methods for nonconvex nonlinear and stochastic programming," MathProg, 2016.

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at the end of the presentation

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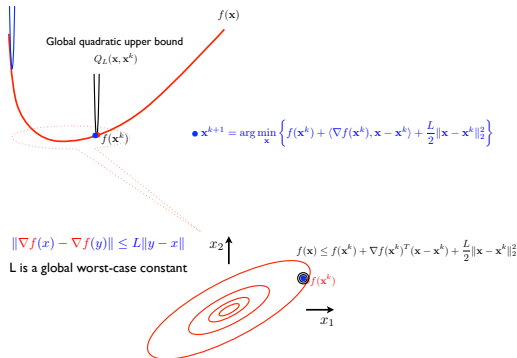
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Worst-case is often too pessimistic

○ GD: $x^{k+1} = x^k - \frac{1}{L} \nabla f(x^k)$



○ Rates are not everything!

- ▶ overall computational effort is what matters
- ▶ constants & implementations are key

○ Knowledge of smoothness, the value of L ,...

- ▶ challenging

○ Must "somehow" adapt to a "different" function

- ▶ online and without knowing L
- ▶ can reduce overall computational effort!

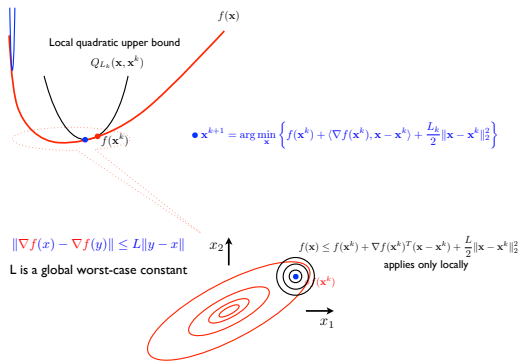
Warmup: f is convex

$$f^* = \min_{x: x \in \mathcal{X}} f(x) \quad (\text{argmin} \rightarrow x^*)$$

A classical approach: Line-search

- Long history: Backtracking, Armijo, steepest descent...

- Universal accelerated gradient method¹



$$f(x^k) - f^* = \mathcal{O} \left(\frac{L_\nu \|x^0 - x^*\|^{1+\nu}}{k^{\frac{1+3\nu}{2}}} \right)$$

- adapts to Hölder smoothness ($\nu \in [0, 1]$)

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L_\nu \|x - y\|_2^\nu$$

- has extensions to primal-dual optimization²
- sets accuracy a priori & monotonic step-sizes

- Not as universal as we wish it to be

- different procedures for stochastic gradients³

¹Y. Nesterov, "Universal Gradient Methods for Convex Optimization Problems," Mathematical Programming, 2015.

²A. Yurtsever, Q. Tran-Dinh, and V. Cevher, "A Universal Primal-Dual Convex Optimization Framework," NeurIPS, 2015.

³S. Vaswani et al., "Painless Stochastic Gradient: Interpolation, Line-Search, and Convergence Rates," NeurIPS, 2019.

A contemporary approach: Online convex optimization (OCO)

Algorithm: A basic online learning problem¹²³

```
1: for  $t = 1, \dots, k$  do  
2:     Player chooses some action  $x^t \in \mathcal{X} \subset \mathbb{R}^p$   
3:     Environment reveals a convex loss  $f_t(\cdot)$   
4:     Player suffers the loss  $f_t(x^t)$   
5: end for
```

- Minimize the total loss vs the best action in hindsight:

$$R(k) = \sum_{t=1}^k f_t(x^t) - \min_{x \in \mathcal{X}} \sum_{t=1}^k f_t(x).$$

- ▶ “somehow” adapts to a “different” function!

- For general convex f_t , optimal regret is sublinear:

$$R(k) = \mathcal{O}(\sqrt{k}).$$

- We can trivially convert regret to rate via $f_t = f$:

$$f\left(\frac{1}{k} \sum_{t=1}^k x^t\right) - f^* \leq \frac{R(k)}{k}.$$

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```

○ One procedure to rule them all...

▶ smooth, non-smooth, stochastic!

○ Not as adaptive as we like in optimization

▶ The “offline” fast rate $1/k^2$ is not immediate

○ Minimize the total loss vs the best action in hindsight:

$$R(k) = \sum_{t=1}^k f_t(x^t) - \min_{x \in \mathcal{X}} \sum_{t=1}^k f_t(x).$$

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The curious case of AdaGrad¹

Algorithm: AdaGrad (scalar)²

```
1: Input: Iterations  $k$ ;  $x_0 \in \mathcal{X}$ 
2: for  $t = 0, \dots, k - 1$  do
3:     Obtain a gradient estimate  $g_t$ 
4:      $\eta_t = D / \left( 2 \sum_{i=1}^t \|g_i\|^2 \right)^{1/2}$ 
5:      $x^{t+1} = P_{\mathcal{X}} \left( x^t - \eta_t g_t \right)$ 
6: end for
7: Output:  $\bar{x}_k = \frac{1}{k} \sum_{t=1}^k x^t$ 
```

- AdaGrad does not need to know smoothness

1. $g_t \in \partial f(x^t)$
2. $g_t = \nabla f(x^t)$
3. $\mathbb{E} g_t = \nabla f(x^t)$ & $\mathbb{E}[\|g - \nabla f(x)\|^2 | x] \leq \sigma^2$

- AdaGrad adapts and achieves optimal regret¹

$$R(k) \leq \sqrt{2D^2 \sum_{t=1}^k \|g_t\|_2^2},$$

where $D = \sup_{x, y \in \mathcal{X}} \|x - y\|_2$.

- When f is L -smooth, AdaGrad output satisfies²

$$\mathbb{E}[f(\bar{x}_k)] - f^* = \mathcal{O} \left(\frac{LD^2}{k} + \frac{\sigma D}{\sqrt{k}} \right).$$

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- Is it an adaptive optimization method?
- Is it a universal optimization method?

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Enter AcceleGrad:¹ Exploiting the linear coupling idea²

Algorithm: AcceleGrad for unconstrained optimization

```
1: Input: Iterations  $k$ ;  $y_0, z_0 \in \mathbb{R}^p$ 
2: for  $t = 0, \dots, k - 1$  do
3:   Obtain a gradient estimate  $g_t$ 
4:    $\alpha_t = \max\left(1, \frac{t+1}{4}\right)$ 
5:    $\eta_t = \frac{1}{\sqrt{G^2 + \sum_{i=0}^t \alpha_i^2 \|g_i\|^2}}$ 
6:    $x^{t+1} = \frac{1}{\alpha_t} y_t + \left(1 - \frac{1}{\alpha_t}\right) z_t,$ 
7:    $z_{t+1} = P_{\mathcal{X}}(z_t - \alpha_t \eta_t g_t)$ 
8:    $y_{t+1} = x^{t+1} - \eta_t g_t$ 
9: end for
10: Output:  $\bar{y}_k \propto \sum_{t=1}^k \alpha_{t-1} y_t$ 
```

◦ AcceleGrad does not need to know smoothness

1. $g_t \in \partial f(x^t)$
2. $g_t = \nabla f(x^t)$
3. $\mathbb{E} g_t = \nabla f(x^t)$ & $\|g\| \leq G$

◦ AcceleGrad output satisfies:¹ $\mathbb{E} f(\bar{y}_k) - f^* =$

1. $\mathcal{O}\left(\frac{GD\sqrt{\log(k)}}{\sqrt{k}}\right)$
2. $\mathcal{O}\left(\frac{DG + LD^2 \log(LD/G)}{k^2}\right)$
3. $\mathcal{O}\left(\frac{GD\sqrt{\log k}}{\sqrt{k}}\right)$

◦ Caveats:

- ▶ needs a bound G on the subgradient norms
- ▶ needs a bound D on $\mathcal{X}$ where the solution lives
- ▶ cannot handle constraints!

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UniXGrad:¹ Universal eXtra Gradient method

Algorithm: UniXGrad

Input: Iterations k ; $y_0 \in \mathcal{X}$; $\alpha_t = t$

1: **for** $t = 0, \dots, k - 1$ **do**

2: $\tilde{y}_t \propto_{\alpha} \alpha_t y_{t-1} + \sum_{i=1}^{t-1} \alpha_i x_i$

3: Obtain a gradient estimate $g_t^{(1)} = g_t(\tilde{y}_t)$

4: $\eta_t = 2D / \sqrt{1 + \sum_{i=1}^{t-1} \alpha_i^2 \left\| g_i^{(1)} - g_i^{(2)} \right\|_*^2}$

5: $x^t = P_{\mathcal{X}} \left(y_{t-1} - \alpha_t \eta_t g_t^{(1)} \right)$

6: $\bar{x}_t \propto_{\alpha} \alpha_t x^t + \sum_{i=1}^{t-1} \alpha_i x_i \rightarrow \text{output}$

7: Obtain a gradient estimate $g_t^{(2)} = g_t(\bar{x}_t)$

8: $y_t = P_{\mathcal{X}} \left(y_{t-1} - \alpha_t \eta_t g_t^{(2)} \right)$

9: **end for**

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² A. Nemirovski, "Prox-method with rate of convergence ... smooth convex-concave saddle point problems," SIOPT, 2005.

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3. $\mathbb{E} g_t(\cdot) = \nabla f(\cdot)$ & $\mathbb{E}[\|g_t(x) - \nabla f(x)\|^2 | x] \leq \sigma^2$

- UniXGrad output satisfies:¹ $\mathbb{E} f(\bar{x}_k) - f^* =$

1. $\frac{6D}{k^2} + \frac{14GD}{\sqrt{k}}$
2. $\frac{20\sqrt{7}D^2L}{k^2}$
3. $\frac{224\sqrt{14}D^2L}{k^2} + \frac{14\sqrt{2}\sigma D}{\sqrt{k}}$

- **First universal and adaptive algorithm**

- ▶ optimal rates in the "offline" setting
- ▶ builds on mirror-prox² & optimistic MD³
- ▶ new online-to-offline conversion lemma¹⁴

f is nonconvex



$$f^* = \min_{x: x \in \mathcal{X}} f(x) \quad (\text{argmin} \rightarrow x^*)$$

Detour: Weak convexity (WeCo) & approximate stationarity¹

- Smooth: Gradient mapping norm

- ▶ $\|G_\eta(x^k)\|^2 = \frac{1}{\eta^2} \|x^k - P_{\mathcal{X}}(x^k - \eta \nabla f(x^k))\|^2$
- ▶ possible to compute

- Non-smooth: Generalized subdifferential distance

- ▶ $\text{dist}(0, \partial(f(x^k) + \delta_{\mathcal{X}}(x^k)))^2$
- ▶ hard in general (even approximately)²³

- f is ρ -weakly convex if $f(x) + \frac{\rho}{2}\|x\|^2$ is convex.

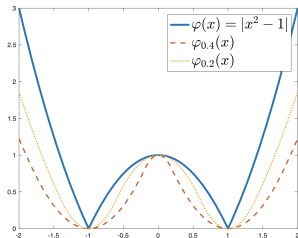


Figure: ME with $f(x) = |x^2 - 1|$, $\mathcal{X} = \mathbb{R}$, and $\hat{v}_t = \mathbb{I}$.¹

- Moreau envelope (ME):

$$\varphi_{1/\rho}(x) = \min_{y \in \mathcal{X}} \left\{ f(y) + \frac{\rho}{2} \|y - x\|^2 \right\}$$

$$\hat{x} \leftarrow \arg \min$$

$$\nabla \varphi_{1/\rho}(x) = \rho(x - \hat{x})$$

- Small $\|\nabla \phi_{1/\rho}(x)\|$ implies near-stationarity:¹

$$\text{dist}(0, \partial(f(x^k) + \delta_{\mathcal{X}}(x^k)))^2 \leq \|\nabla \phi_{1/\rho}(x^k)\|^2$$

- ▶ also implies small $\|G_\eta(x^k)\|^2$ if f is smooth

¹D. Davis and D. Drusvyatskiy, "Stochastic model-based minimization of weakly convex functions," SIOPT, 2019.

³J. Zhang, et al., "On complexity of finding stationary points of nonsmooth nonconvex functions," arXiv:2002.04130, 2020.

³O. Shamir, "Can We Find Near-Approximately-Stationary Points of Nonsmooth Nonconvex Functions?" arXiv:2002.11962, 2020.

The King of all optimization algorithms: Adam¹ (60K+ citations)

Algorithm: (variable metric) Adam

```
1: Input: Iterations  $k$ ;  $x_0 \in \mathcal{X}$ ,  $\beta_{1,2} \in [0, 1]$ 
2: for  $t = 0, \dots, k - 1$  do
3:   Obtain a gradient estimate  $g_t$ 
4:    $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$ 
5:    $\hat{v}_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ 
6:    $x^{t+1} = P_{\mathcal{X}}^{\hat{v}_t^{1/2}} \left( x^t - \alpha_t \hat{v}_t^{-1/2} m_t \right)$ 
7: end for
8: Output:  $x^{t_*^{(k)}}$ :  $t_*(k)$  is randomly chosen in  $\{1, \dots, k\}$ .
```

◦ The King does not need to know smoothness

1. $g_t \in \partial f(x^t)$
2. $g_t = \nabla f(x^t)$
3. $\mathbb{E} g_t = \nabla f(x^t)$ & $\mathbb{E}[\|g - \nabla f(x)\|^2 | x] \leq \sigma^2$

◦ The King adapts and achieves optimal regret³

$$R(k) = \mathcal{O} \left(\sqrt{k} \right),$$

with constant β_1 in OCO.

◦ The King's output satisfies for WeCo⁴

$$\mathbb{E} \|\nabla \phi_{1/\rho}^t(x^{t_*^{(k)}})\|^2 = \mathcal{O} \left(\frac{1}{\sqrt{k}} \right).$$

¹D.P. Kingma and J. Ba, "Adam: A method for stochastic optimization," arXiv:1412.6980, 2014.

²S.J. Reddi, S. Kale, and S. Kumar, "On the convergence of adam and beyond," arXiv:1904.09237, 2019.

³A. Alacaoglu, Y. Malitsky, P. Mertikopoulos, and V. Cevher, "A new regret analysis for adam-type algorithms," ICML 2020

⁴A. Alacaoglu, Y. Malitsky, and V. Cevher, "Convergence of adaptive algorithms for weakly convex constrained optimization," arXiv:2006.06650, 2020.

The King of all optimization algorithms: Adam¹ (60K+ citations)

Algorithm: (variable metric) Adam-type

- 1: **Input:** Iterations k ; $x_0 \in \mathcal{X}$, $\beta_{1,2} \in [0, 1]$
 - 2: **for** $t = 0, \dots, k - 1$ **do**
 - 3: Obtain a gradient estimate g_t
 - 4: $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$
 - 5: $\hat{v}_t = \phi(g_t)$
 - 6: $x^{t+1} = P_{\mathcal{X}}^{\hat{v}_t^{1/2}} \left(x^t - \alpha_t \hat{v}_t^{-1/2} m_t \right)$
 - 7: **end for**
 - 8: **Output:** $x^{t_*(k)}$: $t_*(k)$ is randomly chosen in $\{1, \dots, k\}$.
-

- The King is naked:² AMSGrad

- ▶ $\phi(g_t) = \max(\hat{v}_{t-1}, v_t)$, and $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$
- ▶ F. Orabona: parameterfree.com (Dec 6)

- ~~The King~~ ^{An Adam-type algorithm} does not need to know smoothness

1. $g_t \in \partial f(x^t)$
2. $g_t = \nabla f(x^t)$
3. $\mathbb{E} g_t = \nabla f(x^t)$ & $\mathbb{E}[\|g - \nabla f(x)\|^2 | x] \leq \sigma^2$

- ~~The King~~ ^{An Adam-type algorithm} adapts and achieves optimal regret³

$$R(k) = \mathcal{O} \left(\sqrt{k} \right),$$

with constant β_1 in OCO.

- ~~The King's~~ ^{An Adam-type algorithms'} output satisfies **for WeCo**⁴

$$\mathbb{E} \|\nabla \phi_{1/\rho}^t(x^{t_*(k)})\|^2 = \mathcal{O} \left(\frac{1}{\sqrt{k}} \right).$$

¹D.P. Kingma and J. Ba, "Adam: A method for stochastic optimization," arXiv:1412.6980, 2014.

²S.J. Reddi, S. Kale, and S. Kumar, "On the convergence of adam and beyond," arXiv:1904.09237, 2019.

³A. Alacaoglu, Y. Malitsky, P. Mertikopoulos, and V. Cevher, "A new regret analysis for adam-type algorithms," ICML 2020

⁴A. Alacaoglu, Y. Malitsky, and V. Cevher, "Convergence of adaptive algorithms for weakly convex constrained optimization," arXiv:2006.06650, 2020.

A comparison of algorithms

	GD/SGD	Accelerated GD/SGD	AdaGrad	AcceleGrad/UniXgrad	Adam/AMSGrad
Convex, stochastic	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^1$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^1$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^2$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^{3,4}$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^5$
Convex, deterministic, L -smooth	$\mathcal{O}\left(\frac{1}{k}\right)^1$	$\mathcal{O}\left(\frac{1}{k^2}\right)^1$	$\mathcal{O}\left(\frac{1}{k}\right)^3$	$\mathcal{O}\left(\frac{1}{k^2}\right)^{3,4}$	$\mathcal{O}\left(\frac{1}{k}\right)^6$
Nonconvex, stochastic, L -smooth	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^1$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^1$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^7$	?	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^8$
Nonconvex, deterministic, L -smooth	$\mathcal{O}\left(\frac{1}{k}\right)^1$	$\mathcal{O}\left(\frac{1}{k}\right)^1$	$\mathcal{O}\left(\frac{1}{k}\right)^7$	?	$\mathcal{O}\left(\frac{1}{k}\right)^6$

¹ Lan, First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

² Duchi, Hazan, Singer, Adaptive subgradient methods for online learning and stochastic optimization, JMLR, 2011

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⁴ Kavis, Levy, Bach, Cevher, UniXGrad: A Universal, Adaptive Algorithm with Optimal Guarantees for Constrained Optimization, NeurIPS, 2019

⁵ Reddi, Kale, Kumar, On the convergence of adam and beyond, ICLR, 2018.

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Conclusions

- Simple algorithms automatically adapt to strong convexity under broad assumptions
 - ▶ GD achieves linear rate with $\eta = 1/L^1$
 - ▶ SGD achieves $\mathcal{O}(1/k)$ -rate with $\eta_k = \mathcal{O}(1/k)^2$
 - ▶ PDHG achieves linear rate under metric subregularity³⁴⁵
- Adaptive methods are promising but are not yet truly universal...
 - ▶ Accelegrad/UniXgrad does not adapt to strong convexity
 - ▶ AdaGrad needs a different step-size policy
 - ▶ Adam-type does not adapt to strong convexity
 - ▶ MetaGrad comes close but is not universal yet⁶
- Still seeking one algorithm to rule them all!

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⁵J. Liang, J. Fadili, and G. Peyré, "Convergence rates with inexact non-expansive operators." MathProg, 2016.

⁶T. van Erven, and W.M. Koolen, "Metagrad: Multiple learning rates in online learning." NeurIPS 2016.

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Logistic regression

- Data: a4a
- Oracle: Deterministic

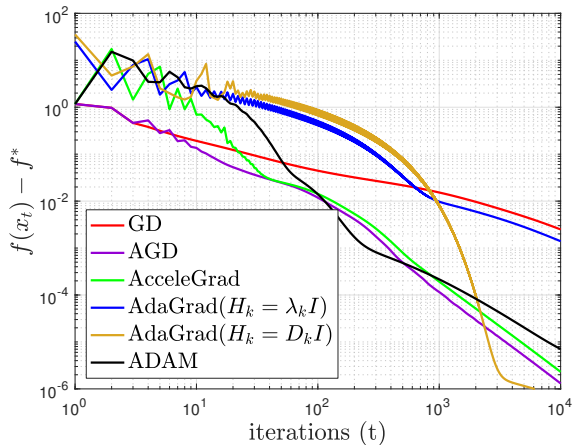


Figure: Logistic regression on a4a

Neural network training: ADAM vs. AcceleGrad

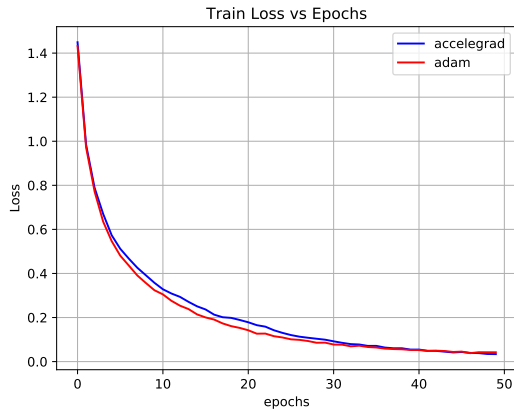


Figure: Resnet classifier optimization (train loss)

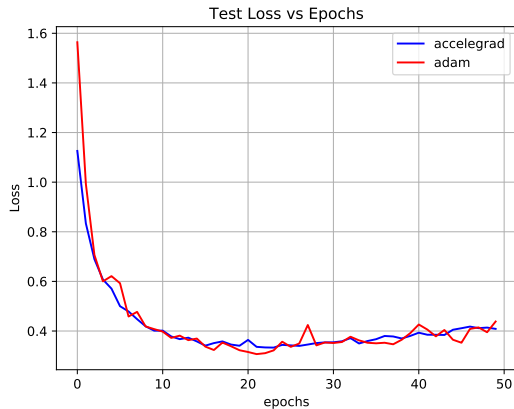


Figure: Resnet classifier optimization (test loss)