On Gradient-Based Optimization: Accelerated, Asynchronous, Distributed and Stochastic

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with Andre Wibisono, Ashia Wilson and Michael Betancourt

Outline

- Variational, Hamiltonian and symplectic perspectives on Nesterov acceleration
- Avoiding saddle points, efficiently
- Stochastically-controlled stochastic gradient

Variational, Hamiltonian and Symplectic Perspectives on Acceleration

with Andre Wibisono, Ashia Wilson and Michael Betancourt

Interplay between Differentiation and Integration

- The 300-yr-old fields: Physics, Statistics
  - cf. Lagrange/Hamilton, Laplace expansions, saddlepoint expansions
- The numerical disciplines
  - e.g.,. finite elements, Monte Carlo

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- The numerical disciplines
  - e.g.,. finite elements, Monte Carlo
- Optimization?

Accelerated gradient descent

Setting: Unconstrained convex optimization

$$\min_{x \in \mathbb{R}^d} f(x)$$

- Classical gradient descent:

$$x_{k+1} = x_k - \beta \nabla f(x_k)$$

  obtains a convergence rate of $O(1/k)$

- Accelerated gradient descent:

$$\begin{aligned} y_{k+1} &= x_k - \beta \nabla f(x_k) \\ x_{k+1} &= (1 - \lambda_k) y_{k+1} + \lambda_k y_k \end{aligned}$$

  obtains the (optimal) convergence rate of $O(1/k^2)$

The acceleration phenomenon

Two classes of algorithms:

- **Gradient methods**
  - Gradient descent, mirror descent, cubic-regularized Newton's method (Nesterov and Polyak '06), etc.
  - Greedy descent methods, relatively well-understood
- **Accelerated methods**
  - Nesterov's accelerated gradient descent, accelerated mirror descent, accelerated cubic-regularized Newton's method (Nesterov '08), etc.
  - Important for both theory (optimal rate for first-order methods) and practice (many extensions: FISTA, stochastic setting, etc.)
  - *Not* descent methods, faster than gradient methods, still mysterious

Accelerated methods: Continuous time perspective

- Gradient descent is discretization of gradient flow

$$\dot{X}_t = -\nabla f(X_t)$$

(and mirror descent is discretization of natural gradient flow)

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$$\ddot{X}_t + \frac{3}{t}\dot{X}_t + \nabla f(X_t) = 0$$

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- These ODEs are obtained by taking continuous time limits. Is there a deeper generative mechanism?

Our work: A general variational approach to acceleration

A systematic discretization methodology

Bregman Lagrangian

Define the **Bregman Lagrangian**:

$$\mathcal{L}(x, \dot{x}, t) = e^{\gamma_t + \alpha_t} \left(D_h(x + e^{-\alpha_t} \dot{x}, x) - e^{\beta_t} f(x) \right)$$

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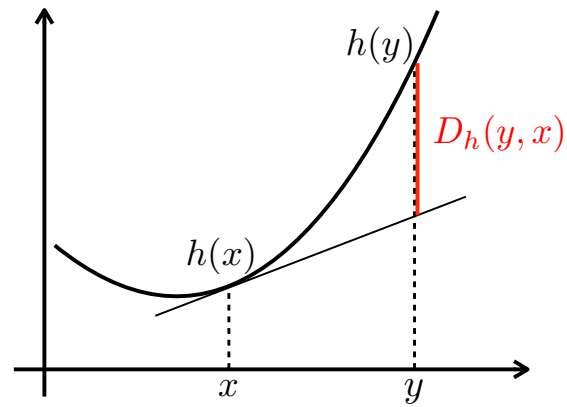
- Function of position x, velocity $\dot{x}$, and time t
- $D_h(y, x) = h(y) - h(x) - \langle \nabla h(x), y - x \rangle$ is the Bregman divergence
- h is the convex distance-generating function



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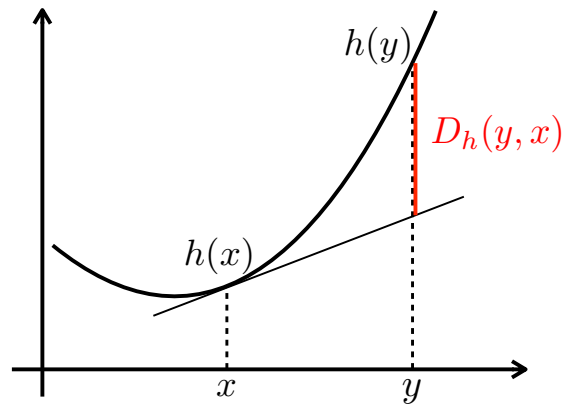

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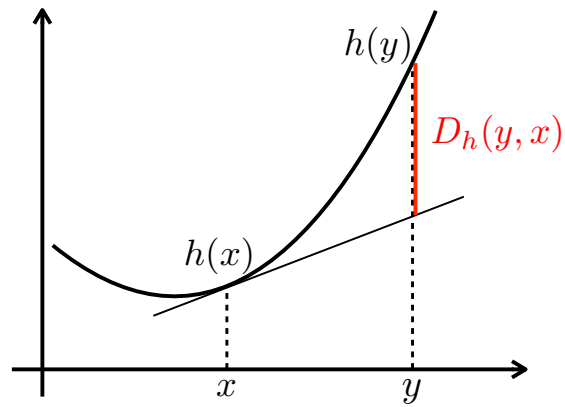

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Define the **Bregman Lagrangian**:

$$\mathcal{L}(x, \dot{x}, t) = e^{\gamma_t - \alpha_t} \left(\frac{1}{2} \|\dot{x}\|^2 - e^{2\alpha_t + \beta_t} f(x) \right)$$

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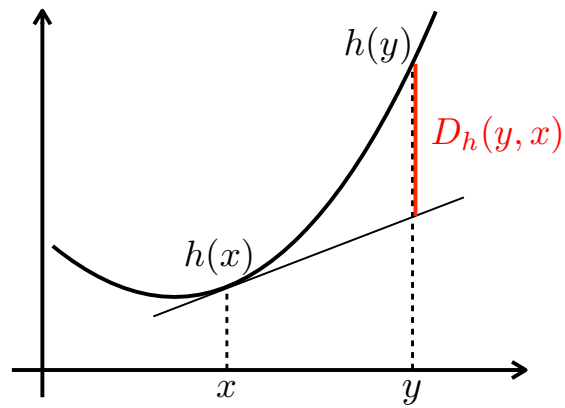
- In Euclidean setting, simplifies to damped Lagrangian



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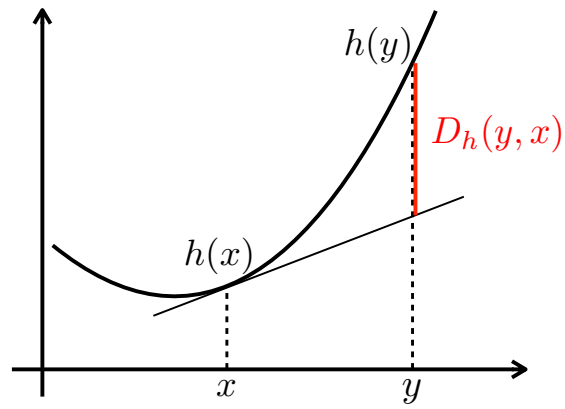

Ideal scaling conditions:

$$\dot{\beta}_t \leq e^{\alpha_t}$$

$$\dot{\gamma}_t = e^{\alpha_t}$$

Bregman Lagrangian

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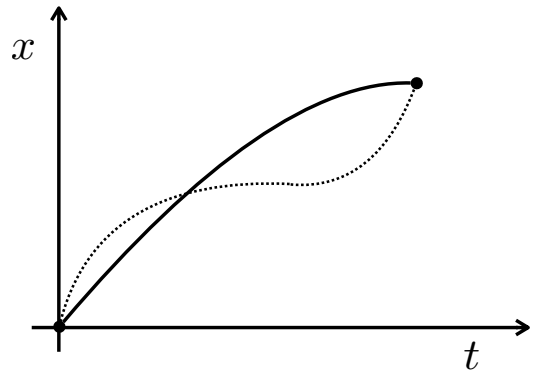
Variational problem over curves:

$$\min_X \int \mathcal{L}(X_t, \dot{X}_t, t)\, dt$$



Optimal curve is characterized by **Euler-Lagrange** equation:

$$\frac{d}{dt} \left\{ \frac{\partial \mathcal{L}}{\partial \dot{x}}(X_t, \dot{X}_t, t) \right\} = \frac{\partial \mathcal{L}}{\partial x}(X_t, \dot{X}_t, t)$$

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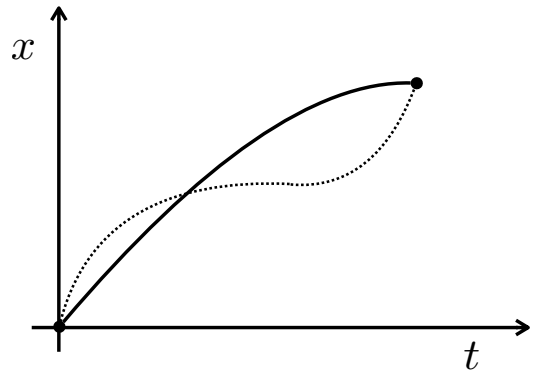

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E-L equation for Bregman Lagrangian under ideal scaling:

$$\ddot{X}_t + (e^{\alpha_t} - \dot{\alpha}_t)\dot{X}_t + e^{2\alpha_t + \beta_t} \left[\nabla^2 h(X_t + e^{-\alpha_t} \dot{X}_t) \right]^{-1} \nabla f(X_t) = 0$$

General convergence rate

Theorem

Theorem Under ideal scaling, the E-L equation has convergence rate

$$f(X_t) - f(x^*) \leq O(e^{-\beta_t})$$

General convergence rate

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Theorem Under ideal scaling, the E-L equation has convergence rate

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Proof. Exhibit a Lyapunov function for the dynamics:

$$\mathcal{E}_t = D_h\left(x^*,\, X_t + e^{-\alpha_t}\dot{X}_t\right) + e^{\beta_t}(f(X_t) - f(x^*))$$

$$\dot{\mathcal{E}}_t = -e^{\alpha_t+\beta_t} D_f(x^*, X_t) + (\dot{\beta}_t - e^{\alpha_t})e^{\beta_t}(f(X_t) - f(x^*)) \;\leq\; 0$$

□

Note: Only requires convexity and differentiability of f, h

Polynomial convergence rate

For $p > 0$, choose parameters:

$$\alpha_t = \log p - \log t$$
$$\beta_t = p \log t + \log C$$
$$\gamma_t = p \log t$$

E-L equation has $O(e^{-\beta_t}) = O(1/t^p)$ convergence rate:

$$\ddot{X}_t + \frac{p+1}{t}\dot{X}_t + Cp^2 t^{p-2}\left[\nabla^2 h\left(X_t + \frac{t}{p}\dot{X}_t\right)\right]^{-1}\nabla f(X_t) = 0$$

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For $p = 2$:

- Recover result of Krichene et al with $O(1/t^2)$ convergence rate
- In Euclidean case, recover ODE of Su et al:
  $\ddot{X}_t + \frac{3}{t}\dot{X}_t + \nabla f(X_t) = 0$

Time dilation property (reparameterizing time)

($p = 2$: accelerated gradient descent)

$$O\left(\frac{1}{t^2}\right): \quad \ddot{X}_t + \frac{3}{t}\dot{X}_t + 4C\left[\nabla^2 h\left(X_t + \frac{t}{2}\dot{X}_t\right)\right]^{-1}\nabla f(X_t) = 0$$

$$\Big\downarrow \quad \text{speed up time: } Y_t = X_{t^{3/2}}$$

$$O\left(\frac{1}{t^3}\right): \quad \ddot{Y}_t + \frac{4}{t}\dot{Y}_t + 9Ct\left[\nabla^2 h\left(Y_t + \frac{t}{3}\dot{Y}_t\right)\right]^{-1}\nabla f(Y_t) = 0$$

($p = 3$: accelerated cubic-regularized Newton's method)

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($p = 3$: accelerated cubic-regularized Newton's method)

- All accelerated methods are traveling the same curve in space-time at different speeds
- Gradient methods don't have this property
  - From gradient flow to rescaled gradient flow: Replace $\frac{1}{2}\|\cdot\|^2$ by $\frac{1}{p}\|\cdot\|^p$

Time dilation for general Bregman Lagrangian

$$O(e^{-\beta_t}): \quad \text{E-L for Lagrangian } \mathcal{L}_{\alpha,\beta,\gamma}$$

$$\Big\downarrow \quad \text{speed up time: } Y_t = X_{\tau(t)}$$

$$O(e^{-\beta_{\tau(t)}}): \quad \text{E-L for Lagrangian } \mathcal{L}_{\tilde{\alpha},\tilde{\beta},\tilde{\gamma}}$$

where

$$\begin{aligned}
\tilde{\alpha}_t &= \alpha_{\tau(t)} + \log \dot{\tau}(t) \\
\tilde{\beta}_t &= \beta_{\tau(t)} \\
\tilde{\gamma}_t &= \gamma_{\tau(t)}
\end{aligned}$$

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\tilde{\gamma}_t &= \gamma_{\tau(t)}
\end{aligned}$$

Question: How to discretize E-L while preserving the convergence rate?

Discretizing the dynamics (naive approach)

Write E-L as a system of first-order equations:

$$Z_t = X_t + \frac{t}{p}\dot{X}_t$$

$$\frac{d}{dt}\nabla h(Z_t) = -Cpt^{p-1}\nabla f(X_t)$$

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Euler discretization with time step $\delta > 0$ (i.e., set $x_k = X_t$, $x_{k+1} = X_{t+\delta}$):

$$x_{k+1} = \frac{p}{k+p}z_k + \frac{k}{k+p}x_k$$

$$z_k = \arg\min_z \left\{ Cpk^{(p-1)}\langle \nabla f(x_k), z\rangle + \frac{1}{\epsilon}D_h(z, z_{k-1}) \right\}$$

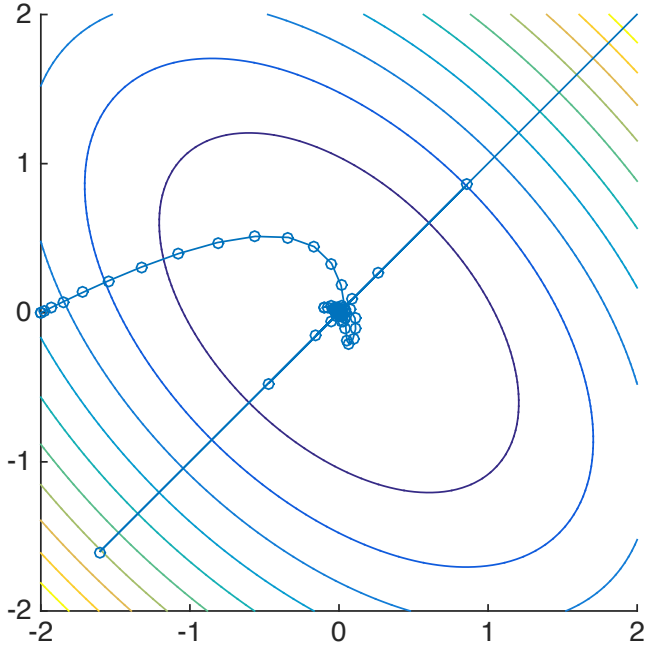
with step size $\epsilon = \delta^p$, and $k^{(p-1)} = k(k+1)\cdots(k+p-2)$ is the rising factorial

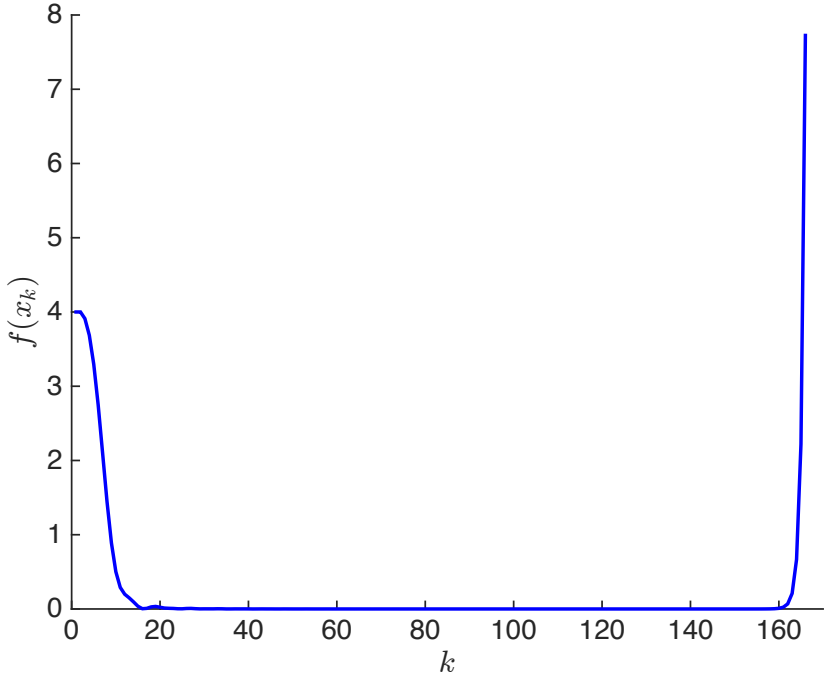
Naive discretization doesn't work

$$x_{k+1} = \frac{p}{k+p} z_k + \frac{k}{k+p} x_k$$

$$z_k = \arg\min_z \left\{ Cpk^{(p-1)} \langle \nabla f(x_k), z \rangle + \frac{1}{\epsilon} D_h(z, z_{k-1}) \right\}$$

Cannot obtain a convergence guarantee, and empirically unstable





Modified discretization

Introduce an auxiliary sequence y_k:

$$x_{k+1} = \frac{p}{k+p} z_k + \frac{k}{k+p} y_k$$

$$z_k = \arg\min_z \left\{ Cpk^{(p-1)} \langle \nabla f(y_k), z \rangle + \frac{1}{\epsilon} D_h(z, z_{k-1}) \right\}$$

Sufficient condition: $\langle \nabla f(y_k), x_k - y_k \rangle \geq M \epsilon^{\frac{1}{p-1}} \|\nabla f(y_k)\|_*^{\frac{p}{p-1}}$

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Sufficient condition: $\langle \nabla f(y_k), x_k - y_k \rangle \geq M \epsilon^{\frac{1}{p-1}} \|\nabla f(y_k)\|_*^{\frac{p}{p-1}}$

Assume h is uniformly convex: $D_h(y, x) \geq \frac{1}{p}\|y - x\|^p$

Theorem

Theorem

$$f(y_k) - f(x^*) \leq O\left(\frac{1}{\epsilon k^p}\right)$$

Note: Matching convergence rates $1/(\epsilon k^p) = 1/(\delta k)^p = 1/t^p$

Proof using generalization of Nesterov's estimate sequence technique

Accelerated higher-order gradient method

$$x_{k+1} = \frac{p}{k+p} z_k + \frac{k}{k+p} y_k$$

$$y_k = \arg\min_y \left\{ f_{p-1}(y; x_k) + \frac{2}{\epsilon p} \|y - x_k\|^p \right\} \quad \leftarrow O\left(\frac{1}{\epsilon k^{p-1}}\right)$$

$$z_k = \arg\min_z \left\{ Cpk^{(p-1)} \langle \nabla f(y_k), z \rangle + \frac{1}{\epsilon} D_h(z, z_{k-1}) \right\}$$

If $\nabla^{p-1} f$ is $(1/\epsilon)$-Lipschitz and h is uniformly convex of order p, then:

$$f(y_k) - f(x^*) \leq O\left(\frac{1}{\epsilon k^p}\right) \quad \leftarrow \text{ accelerated rate}$$

$p = 2$: Accelerated gradient/mirror descent

$p = 3$: Accelerated cubic-regularized Newton's method (Nesterov '08)

$p \geq 2$: Accelerated higher-order method

Recap: Gradient vs. accelerated methods

How to design dynamics for minimizing a convex function f?

Rescaled gradient flow

$$\dot{X}_t = -\nabla f(X_t) \,/\, \|\nabla f(X_t)\|_*^{\frac{p-2}{p-1}}$$

$$O\left(\frac{1}{t^{p-1}}\right)$$

Higher-order gradient method

$O\left(\frac{1}{\epsilon k^{p-1}}\right)$ when $\nabla^{p-1} f$ is $\frac{1}{\epsilon}$-Lipschitz

matching rate with $\epsilon = \delta^{p-1} \Leftrightarrow \delta = \epsilon^{\frac{1}{p-1}}$

Recap: Gradient vs. accelerated methods

How to design dynamics for minimizing a convex function f?

Rescaled gradient flow	Polynomial Euler-Lagrange equation
$\dot{X}_t = -\nabla f(X_t) \,/\, \|\nabla f(X_t)\|_*^{\frac{p-2}{p-1}}$	$\ddot{X}_t + \frac{p+1}{t}\dot{X}_t + t^{p-2}\left[\nabla^2 h\left(X_t + \frac{t}{p}\dot{X}_t\right)\right]^{-1}\nabla f(X_t) =$
$O\left(\frac{1}{t^{p-1}}\right)$	$O\left(\frac{1}{t^p}\right)$
Higher-order gradient method	**Accelerated higher-order method**
$O\left(\frac{1}{\epsilon k^{p-1}}\right)$ when $\nabla^{p-1} f$ is $\frac{1}{\epsilon}$-Lipschitz	$O\left(\frac{1}{\epsilon k^{p}}\right)$ when $\nabla^{p-1} f$ is $\frac{1}{\epsilon}$-Lipschitz
matching rate with $\epsilon = \delta^{p-1} \Leftrightarrow \delta = \epsilon^{\frac{1}{p-1}}$	matching rate with $\epsilon = \delta^{p} \Leftrightarrow \delta = \epsilon^{\frac{1}{p}}$

Towards A Symplectic Perspective

- If initialized close enough, diminishing gradient flow will relax to an optimum quickly

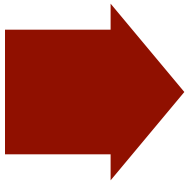
$$\frac{\mathrm{d}q}{\mathrm{d}t} = -\frac{C}{t}\nabla f(q)$$

Towards A Symplectic Perspective

- We can construct physical systems that will rapidly evolve into the neighborhood of the optimum, but the inertia can slow relaxation once we get there

$$L(q, v, f(q), t)$$

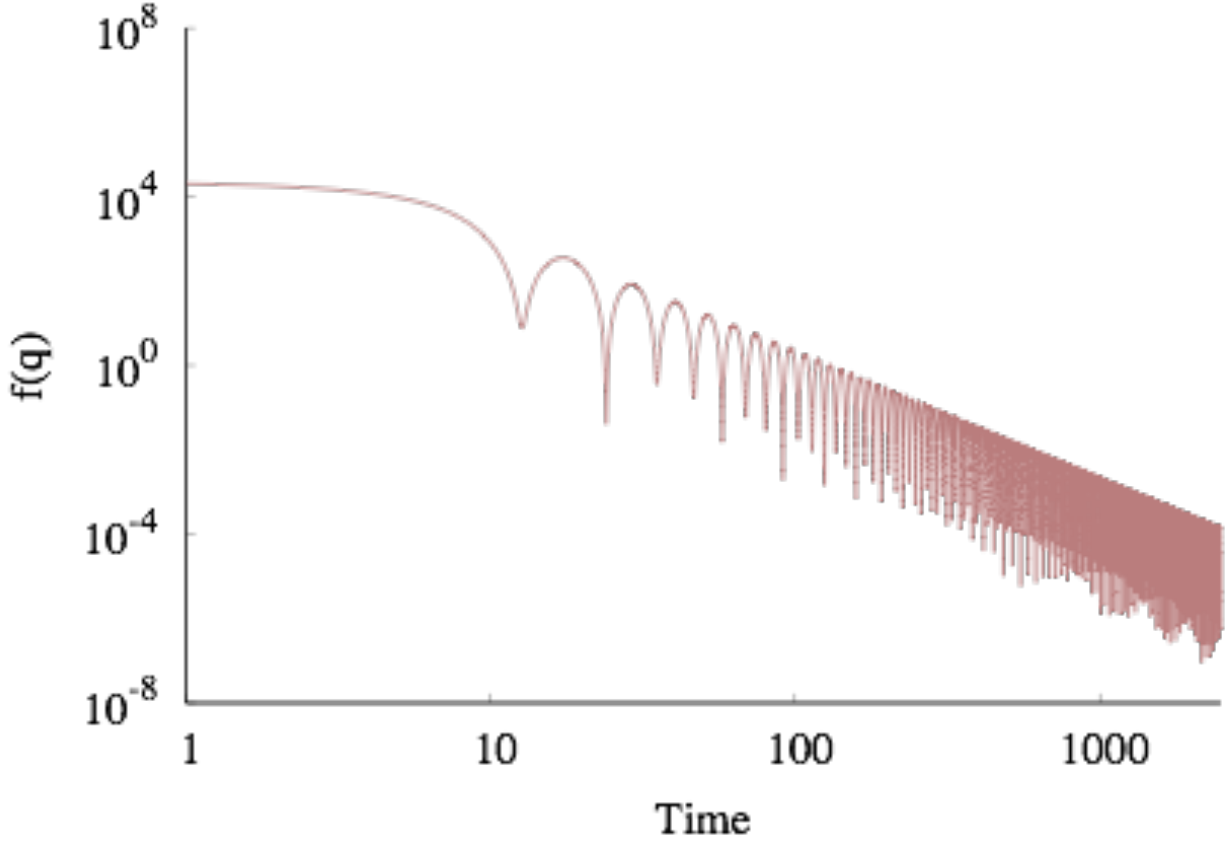
$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial v} = \frac{\partial L}{\partial q}$$



$$\frac{\mathrm{d}q}{\mathrm{d}t} = v$$

$$\frac{\mathrm{d}v}{\mathrm{d}t} = g(q, v, t)$$

Towards A Symplectic Perspective



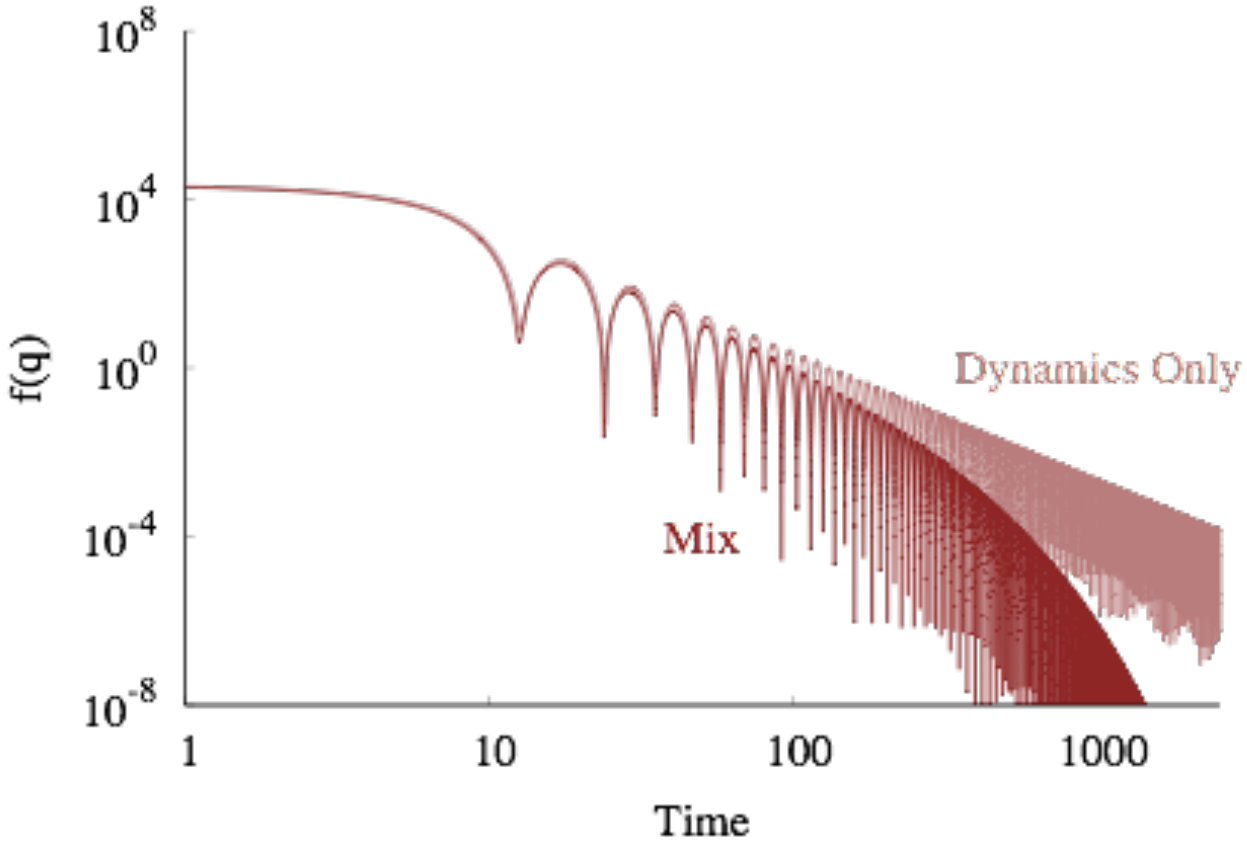
Towards A Symplectic Perspective

- Can a mixture of these flows yield rapid convergence to the optimum in both regimes?

$$\frac{\mathrm{d}q}{\mathrm{d}t} = v \quad -\delta \frac{C}{t} \nabla f(q)$$

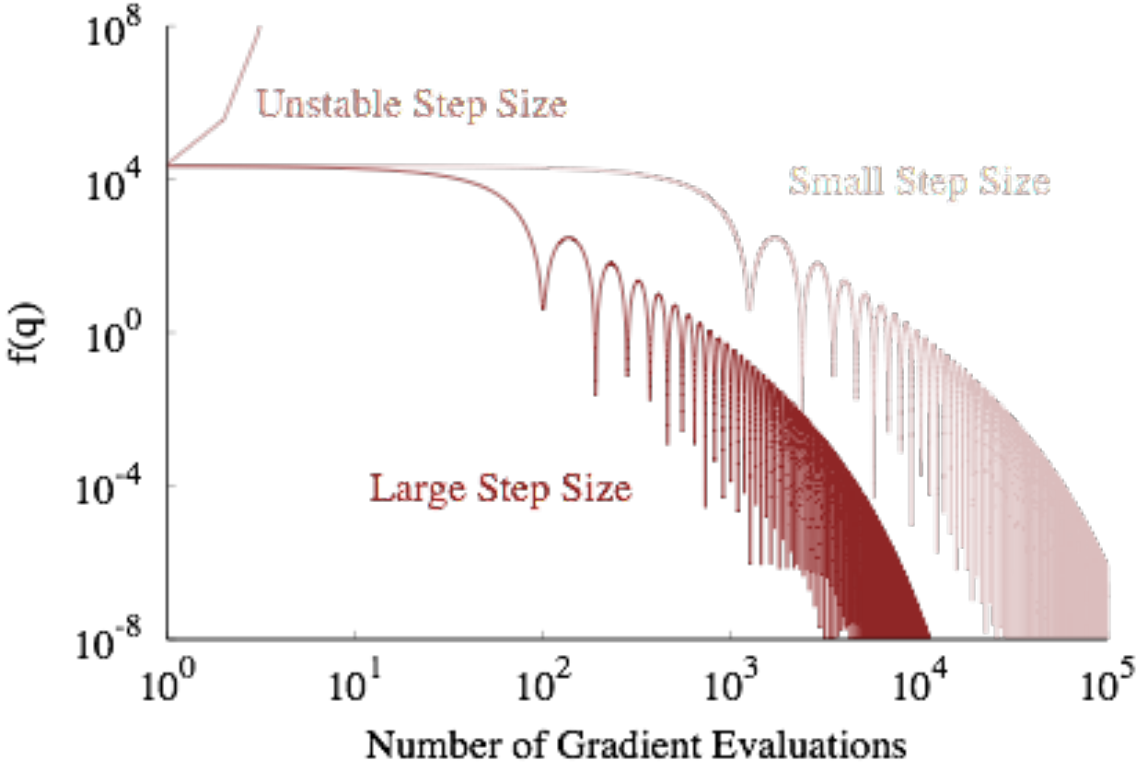
$$\frac{\mathrm{d}v}{\mathrm{d}t} = g(q, v, t)$$

Towards A Symplectic Perspective



Towards A Symplectic Perspective

- Speed also depends on the discretization



Towards A Symplectic Perspective

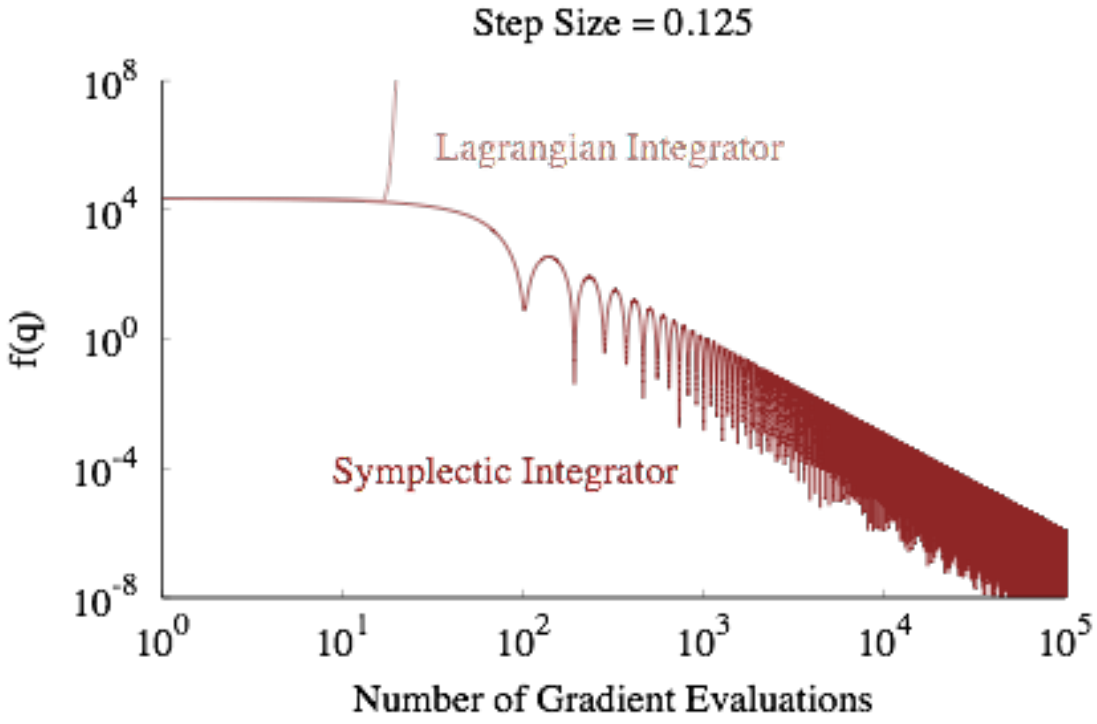
- Discretization of the Lagrangian dynamics, however, is fragile and requires small step sizes.
- We can build more robust solutions by taking a Legendre transform and considering a *Hamiltonian* formalism:

$$L(q, v, t) \rightarrow H(q, p, t, \mathcal{E})$$

$$\left(\frac{\mathrm{d}q}{\mathrm{d}t}, \frac{\mathrm{d}v}{\mathrm{d}t}\right) \rightarrow \left(\frac{\mathrm{d}q}{\mathrm{d}\tau}, \frac{\mathrm{d}p}{\mathrm{d}\tau}, \frac{\mathrm{d}t}{\mathrm{d}\tau}, \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}\tau}\right)$$

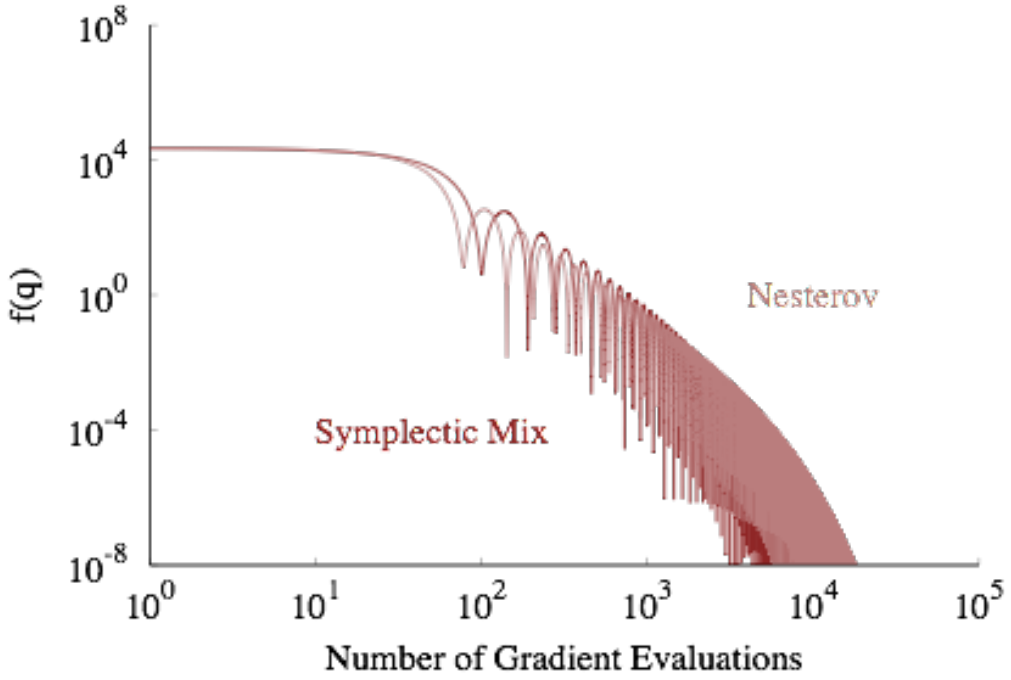
Towards A Symplectic Perspective

- The Hamiltonian perspective admits *symplectic integrators* which are accurate and stable even for large step sizes



Towards A Symplectic Perspective

- Exploiting this stability yields algorithms with state-of-the-art performance, and perhaps even more:



Part II

Avoiding Saddlepoints, Efficiently

with Chi Jin, Rong Ge, Praneeth Netrapalli and Sham Kakade

Definitions and Algorithm

Function $f(\cdot)$ is ρ-**Hessian Lipschitz** if

$$\forall \mathbf{x}_1, \mathbf{x}_2, \ \|\nabla^2 f(\mathbf{x}_1) - \nabla^2 f(\mathbf{x}_2)\| \leq \rho \|\mathbf{x}_1 - \mathbf{x}_2\|.$$

Point $\mathbf{x}$ is an ϵ-**second-order stationary point** (ϵ-SOSP) if

$$\|\nabla f(\mathbf{x})\| \leq \epsilon, \qquad \text{and} \qquad \lambda_{\min}(\nabla^2 f(\mathbf{x})) \geq -\sqrt{\rho\epsilon}$$

Perturbed Gradient Descent (PGD)

1. **for** $t = 0, 1, \ldots$ **do**
2. **if** perturbation condition holds **then**
3. $\mathbf{x}_t \leftarrow \mathbf{x}_t + \xi_t, \qquad \xi_t$ uniformly $\sim \mathbb{B}_0(r)$
4. $\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t - \eta \nabla f(\mathbf{x}_t)$

Only adds perturbation when $\nabla f(\mathbf{x}_t) \leq \epsilon$, and no more than once per T steps.

Main Result

PGD Converges to SOSP (This Work)

For ℓ-smooth and ρ-Hessian Lipschitz function f, PGD with $\eta = O(1/\ell)$ and proper choice of r, T w.h.p. finds ϵ-SOSP in iterations:

$$\tilde{O}\left(\frac{\ell(f(\mathbf{x}_0) - f^\star)}{\epsilon^2}\right)$$

*Dimension dependence in iteration is $\log^4(d)$ (almost dimension free).

	GD(Nestrov 1998)	**PGD**(This Work)
Assumptions	ℓ-grad-Lip	ℓ-grad-Lip + ρ-Hessian-Lip
Guarantees	ϵ-FOSP	ϵ-SOSP
Iterations	$2\ell(f(\mathbf{x}_0) - f^\star)/\epsilon^2$	$\tilde{O}(\ell(f(\mathbf{x}_0) - f^\star)/\epsilon^2)$

Part III

Stochastically-Controlled Stochastic Gradient

with Lihua Lei

Setup

Task: minimizing a composite objective:

$$\min_{x \in \mathbb{R}^d} f(x) = \frac{1}{n} \sum_{i \in [n]} f_i(x)$$

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$$\frac{\mu}{2}\|x - y\|^2 \leq f_i(x) - f_i(y) - \langle \nabla f_i(y), x - y \rangle \leq \frac{L}{2}\|x - y\|^2$$

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- $\mu = 0$: non-strongly convex case;
- $\mu > 0$: strongly convex case; $\kappa \triangleq L/\mu$.

Computation Complexity

- Accessing $(f_i(x), \nabla f_i(x))$ incurs one unit of cost;
- Given $\epsilon > 0$, let $T(\epsilon)$ be the minimum cost to achieve

$$\mathbb{E}\left(f(x_{T(\epsilon)}) - f(x^*)\right) \leq \epsilon;$$

- Worst-case analysis: bound $T(\epsilon)$ almost surely, e.g.,

$$T(\epsilon) = O\left((n + \kappa) \log \frac{1}{\epsilon}\right) \qquad \text{(SVRG)}.$$

SVRG Algorithm

SVRG: (within an epoch)

$\mathcal{I} \leftarrow [n]$

$g \leftarrow \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} f_i'(x_0)$

$m \leftarrow n$

Generate $N \sim U([m])$

for $k = 1, 2, \cdots, N$ **do**

    Randomly pick $i \in [n]$

    $\nu \leftarrow f_i'(x) - f_i'(x_0) + g$

    $x \leftarrow x - \eta\nu$

end for

Analysis

	General Convex	Strongly Convex
Nesterov's AGD	$\frac{n}{\sqrt{\epsilon}}$	$n\sqrt{\kappa}\log\frac{1}{\epsilon}$
SGD	$\frac{1}{\epsilon^2}$	$\frac{\kappa}{\epsilon}\log\frac{1}{\epsilon}$
SVRG	-	$(n+\kappa)\log\frac{1}{\epsilon}$
Katyusha	$\frac{n}{\sqrt{\epsilon}}$	$(n+\sqrt{n\kappa})\log\frac{1}{\epsilon}$

- All above results are from worst-case analysis;
- SGD is the only method with complexity free of n; however, the stepsize η depends on the unknown $\|x_0 - x^*\|^2$ and the total number of epochs T.

Average-Case Analysis

- Instead of bounding $T(\epsilon)$, one can bound $\mathbb{E}T(\epsilon)$;
- Evidence from other areas that average-case analysis can give much better complexity bounds than worst-case analysis.

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- Instead of bounding $T(\epsilon)$, one can bound $\mathbb{E}T(\epsilon)$;
- Evidence from other areas that average-case analysis can give much better complexity bounds than worst-case analysis.
- Goal: design an efficient algorithm such that
  - $\mathbb{E}T(\epsilon)$ is independent of n;
  - $\mathbb{E}T(\epsilon)$ is smaller than the worst-case bounds.

Average-Case Analysis

An algorithm is *tuning-friendly* if:

- the stepsize η is the only parameter to tune;
- η is a constant which only depends on L and μ.

	General Convex	Strongly Convex	Tuning-friendly
SGD	$\frac{1}{\epsilon^2}$	$\frac{\kappa}{\epsilon}\log\frac{1}{\epsilon}$	No
SCSG	$\frac{1}{\epsilon^2}\wedge\frac{n}{\epsilon}$	$\left(\frac{1}{\epsilon}\wedge n+\kappa\right)\log\frac{1}{\epsilon}$	Yes
SCSG+	$\frac{1}{\epsilon}\log\left(\frac{1}{\epsilon}\wedge n\right)+\frac{\log n}{n\epsilon^2}$	$\frac{1}{\epsilon}+\frac{\kappa}{\epsilon^\alpha}(\alpha\ll 1)$	Yes
SCSG+	$\frac{1}{\epsilon}\sqrt{\log\left(\frac{1}{\epsilon}\wedge n\right)}+\frac{\sqrt{\log n}}{\sqrt{n}\epsilon^{\frac{3}{2}}}$	$\sqrt{\frac{\kappa}{\epsilon}}+\kappa$	No

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SCSG/SCSG+: Algorithm

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SCSG/SCSG+: Algorithm

In epoch j,

- SCSG fixes $B_j \equiv B(\epsilon)$;
- Explicit forms of $B(\epsilon)$ are given in both non-strongly convex cases and strongly convex cases;
- SCSG+ uses an geometrically increasing sequence

$$B_j = \lceil B_0 b^j \wedge n \rceil$$

Conclusion

- SCSG/SCSG+ saves computation costs on average by avoiding calculating the full gradient;
- SCSG/SCSG+ also saves communication costs in the distributed system by avoiding sampling a gradient from the whole dataset;
- SCSG/SCSG+ are able to achieve an approximate optimum with potentially less than a single pass through the data;
- The average computation cost of SCSG+ beats the oracle lower bounds from worst-case analysis.