On Computational Thinking, Inferential Thinking and "Data Science"

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What Is the Big Data Phenomenon?

- Science in confirmatory mode (e.g., particle physics)
 inferential issue: massive number of nuisance variables
- Science in exploratory mode (e.g., astronomy, genomics)
 inferential issue: massive number of hypotheses
- Measurement of human activity, particularly online activity, is generating massive datasets that can be used (e.g.) for personalization and for creating markets
 - *inferential issues*: many, including heterogeneity, unknown sampling frames, compound loss function

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- "It should only improve as we collect more data; in particular it shouldn't slow down"
- "There are serious privacy concerns of course, and they vary across the clients"

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- What I mean by computational thinking
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- Big Data analysis requires a thorough blending of computational thinking and inferential thinking
- What I mean by computational thinking
 - abstraction, modularity, scalability, robustness, etc.
- Inferential thinking means (1) considering the realworld phenomenon behind the data, (2) considering the sampling pattern that gave rise to the data, and (3) developing procedures that will go "backwards" from the data to the underlying phenomenon

The Challenges are Daunting

- The core theories in computer science and statistics developed separately and there is an oil and water problem
- Core statistical theory doesn't have a place for runtime and other computational resources
- Core computational theory doesn't have a place for statistical risk

Outline

- Inference under privacy constraints
- Inference under communication constraints
- The variational perspective

Part I: Inference and Privacy

with John Duchi and Martin Wainwright

Privacy and Data Analysis

- Individuals are not generally willing to allow their personal data to be used without control on how it will be used and now much privacy loss they will incur
- "Privacy loss" can be quantified via differential privacy
- We want to trade privacy loss against the value we obtain from "data analysis"
- The question becomes that of quantifying such value and juxtaposing it with privacy loss

Privacy

query database

Privacy

query database $\tilde{\theta}$

Privacy



Privacy



Privacy







Classical problem in differential privacy: show that $\hat{\theta}$ and $\tilde{\theta}$ are close under constraints on Q









Classical problem in statistical theory: show that $\tilde{\theta}$ and θ are close under constraints on S

Privacy and Inference



The privacy-meets-inference problem: show that θ and $\hat{\theta}$ are close under constraints on Q and on S

Background on Inference

- In the 1930's, Wald laid the foundations of statistical decision theory
- Given a family of distributions *P*, a parameter θ(P) for each P ∈ P, an estimator θ̂, and a loss l(θ̂, θ(P)), define the risk:

$$R_P(\hat{\theta}) := \mathbb{E}_P\left[l(\hat{\theta}, \theta(P))\right]$$

Background on Inference

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$$R_P(\hat{\theta}) := \mathbb{E}_P\left[l(\hat{\theta}, \theta(P))\right]$$

• Minimax principle [Wald, '39, '43]: choose estimator minimizing worst-case risk:

$$\sup_{P \in \mathcal{P}} \mathbb{E}_P\left[l(\hat{\theta}, \theta(P))\right]$$

Local Privacy



Local Privacy



Individuals $i \in \{1, \ldots, n\}$ with private data $X_i \stackrel{\text{iid}}{\sim} P$ Estimator $Z_1^n \mapsto \widehat{\theta}(Z_1^n)$

Differential Privacy







Given Z, cannot reliably discriminate between x and x'

Private Minimax Risk

- Parameterheta(P) of distribution
- Family of distributions $\, {\cal P} \,$
- Loss ℓ measuring error
- Family \mathcal{Q}_{lpha} of private channels

lpha -private Minimax risk

$$\mathfrak{M}_{n}(\theta(\mathcal{P}), \ell, \alpha) := \inf_{\substack{Q \in \mathcal{Q}_{\alpha} \ \widehat{\theta} \ P \in \mathcal{P}}} \inf_{\substack{P \in \mathcal{P} \ P \in \mathcal{P}}} \mathbb{E}_{P,Q} \left[\ell(\widehat{\theta}(Z_{1}^{n}), \theta(P)) \right]$$

Best α -private channel

Minimax risk under privacy constraint

Vignette: Private Mean Estimation

Example: estimate reasons for hospital visits Patients admitted to hospital for substance abuse Estimate prevalence of different substances

 $\begin{array}{c} \begin{array}{c} \text{I} \quad \text{Alcohol} \\ \hline & \text{Cocaine} \\ \hline & \text{O} \quad \text{Heroin} \\ \hline & 0 \quad \text{Cannabis} \\ \hline & 0 \quad \text{LSD} \\ \hline & 0 \quad \text{Amphetamines} \end{array} \end{array} \begin{array}{c} \theta_1 &= .45 \\ \theta_2 &= .32 \\ \theta_3 &= .16 \\ \theta_4 &= .20 \\ \theta_5 &= .00 \\ \theta_6 &= .02 \end{array}$

Vignette: Mean Estimation

Consider estimation of mean $\theta(P) := \mathbb{E}_P[X] \in \mathbb{R}^d$, with errors measured in ℓ_{∞} -norm, for

 $\mathcal{P}_d := \{ \text{distributions } P \text{ supported on } [-1,1]^d \}$

Proposition:

Minimax rate

$$\mathfrak{M}_n(\mathcal{P}_d, \left\|\cdot\right\|_{\infty}) \asymp \min\left\{1, \frac{\sqrt{\log d}}{\sqrt{n}}\right\}$$

(achieved by sample mean)

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Proposition:

Private minimax rate for $\alpha = O(1)$ $\mathfrak{M}_n(\mathcal{P}_d, \|\cdot\|_{\infty}, \alpha) \asymp \min\left\{1, \frac{\sqrt{d\log d}}{\sqrt{n\alpha^2}}\right\}$

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Note: Effective sample size $n \mapsto n\alpha^2/d$

Optimal mechanism?



$$Z = X + W = \begin{bmatrix} 1 \\ 1 \end{bmatrix} +$$

Non-private observation

Idea 1: add independent noise (e.g. Laplace mechanism)

[Dwork et al. 06]

Problem: magnitude much too large (this is unavoidable: *provably sub-optimal*)
Optimal mechanism



Non-private observation

Optimal mechanism



Optimal mechanism



Empirical evidence



Estimate proportion of emergency room visits involving different substances

Data source: Drug Abuse Warning Network

Additional Examples

- Fixed-design regression
- Convex risk minimization
- Multinomial estimation
- Nonparametric density estimation
- Almost always, the effective sample size reduction is:

$$n\mapsto rac{nlpha^2}{d}$$

Part III: Inference and Compression

with Yuchen Zhang, John Duchi and Martin Wainwright

Communication Constraints

- Large data necessitates distributed storage
- Independent data collection (e.g., hospitals)
- Privacy



Setting: each of magents has sample of size n

$$X^i = (X_1^i, X_2^i, \dots, X_n^i)$$

Messages Z_i to fusion center

Question: tradeoffs between communication and statistical utility?

[Yao 79; Abelson 80; Tsitsiklis and Luo 87; Han & Amari 98; Tatikonda & Mitter 04; ...]

Minimax Communication

Central object of study:

- Parameter heta(P) of distribution
- Family of distributions ${\cal P}$
- Loss $\left\|\cdot\right\|_2^2$

Constrained to be $\leq B$ bits



Minimax Communication



Consider estimation in normal location family, $heta \in [-1,1]^d$

$$X_j^i \stackrel{\mathrm{iid}}{\sim} \mathsf{N}(\theta, \sigma^2 I_{d \times d})$$



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Theorem: when each agent has sample of size n

Minimax rate

$$\mathbb{E}[\|\widehat{\theta}(X^1,\ldots,X^m) - \theta\|_2^2] \asymp \frac{\sigma^2 d}{nm}$$

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Theorem: when each agent has sample of size n

Minimax rate with *B*-bounded communication

$$\frac{d}{B \wedge d} \frac{1}{\log m} \frac{\sigma^2 d}{nm} \lesssim \mathfrak{M}_n(\mathcal{N}_d, B) \lesssim \frac{d\log m}{B \wedge d} \frac{\sigma^2 d}{nm}$$

X

bits

Consider estimation in normal
location family,
$$\theta \in [-1,1]^d$$

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Minimax rate with B-bounded communication

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Consequence: each sends $\approx d$ bits for optimal estimation

Computation and Inference

 How does inferential quality trade off against classical computational resources such as time and space?

Computation and Inference

- How does inferential quality trade off against classical computational resources such as time and space?
- Hard!

Computation and Inference: Mechanisms and Bounds

- Tradeoffs via convex relaxations
 - linking runtime to convex geometry and risk to convex geometry
- Tradeoffs via concurrency control
 - optimistic concurrency control
- Bounds via optimization oracles
 - number of accesses to a gradient as a surrogate for computation
- Bounds via communication complexity
- Tradeoffs via subsampling
 - bag of little bootstraps, variational consensus Monte Carlo

A Variational Framework for Accelerated Methods in Optimization

with Andre Wibisono and Ashia Wilson

July 12, 2016

Accelerated gradient descent

Setting: Unconstrained convex optimization

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

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Classical gradient descent:

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obtains a convergence rate of O(1/k)

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Accelerated gradient descent:

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

$$x_{k+1} = (1 - \lambda_k) y_{k+1} + \lambda_k y_k$$

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

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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

- Analysis using Nesterov's estimate sequence technique
- Common interpretation as "momentum methods" (Euclidean case)

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- Common interpretation as "momentum methods" (Euclidean case)
- Many proposed explanations:
 - Chebyshev polynomial (Hardt '13)
 - Linear coupling (Allen-Zhu, Orecchia '14)
 - Optimized first-order method (Drori, Teboulle '14; Kim, Fessler '15)
 - Geometric shrinking (Bubeck, Lee, Singh '15)
 - Universal catalyst (Lin, Mairal, Harchaoui '15)
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But only for strongly convex functions, or first-order methods

Question: What is the underlying mechanism that generates acceleration (including for higher-order methods)?

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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 Su, Boyd, Candes '14: Continuous time limit of accelerated gradient descent is a second-order ODE

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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

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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• 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
- f is the convex objective function
- $\alpha_t, \beta_t, \gamma_t \in \mathbb{R}$ are arbitrary smooth functions



Define the Bregman Lagrangian:

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

- 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
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Ideal scaling conditions:

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



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



Optimal curve is characterized by Euler-Lagrange equation:

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

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E-L equation for Bregman Lagrangian under ideal scaling:

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

General convergence rate

Theorem

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

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

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Proof. Exhibit a Lyapunov function for the dynamics:

$$\begin{aligned} \mathcal{E}_t &= D_h\left(x^*, X_t + e^{-\alpha_t} \dot{X}_t\right) + e^{\beta_t}(f(X_t) - f(x^*)) \\ \dot{\mathcal{E}}_t &= -e^{\alpha_t + \beta_t} D_f(x^*, X_t) + (\dot{\beta}_t - e^{\alpha_t}) e^{\beta_t}(f(X_t) - f(x^*)) \leq 0 \end{aligned}$$

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 $O(e^{-eta_t}) = O(1/t^p)$ convergence rate:

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

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For p = 2:

 Recover result of Krichene et al with O(1/t²) 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)

Time dilation property (reparameterizing time)

- 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

$$O(e^{-eta_t})$$
: E-L for Lagrangian $\mathcal{L}_{lpha,eta,\gamma}$
 \downarrow speed up time: $Y_t = X_{ au(t)}$
 $O(e^{-eta_{ au(t)}})$: E-L for Lagrangian $\mathcal{L}_{ ildelpha, ildeeta, ilde\gamma}$

where

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

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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:

$$Z_t = X_t + \frac{t}{\rho} \dot{X}_t$$
$$\frac{d}{dt} \nabla h(Z_t) = -C\rho t^{\rho-1} \nabla f(X_t)$$

Discretizing the dynamics (naive approach)

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

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

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

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

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

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

Cannot obtain a convergence guarantee, and empirically unstable



Modified discretization

Introduce an auxiliary sequence y_k :

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

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

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Sufficient condition: $\langle \nabla f(y_k), x_k - y_k \rangle \ge M \epsilon^{\frac{1}{p-1}} \| \nabla f(y_k) \|_*^{\frac{p}{p-1}}$ Assume *h* is uniformly convex: $D_h(y, x) \ge \frac{1}{p} \| y - x \|^p$

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

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

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

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

Higher-order gradient update

Higher-order Taylor approximation of f:

$$f_{p-1}(y;x) = f(x) + \langle
abla f(x), y-x
angle + \cdots + rac{1}{(p-1)!}
abla^{p-1} f(x)(y-x)^{p-1}$$

Higher-order gradient update:

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

Higher-order gradient update

Higher-order Taylor approximation of *f* :

$$f_{p-1}(y;x) = f(x) + \langle
abla f(x), y-x
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Higher-order gradient update:

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

Assume f is smooth of order p - 1:

$$\|
abla^{p-1}f(y)-
abla^{p-1}f(x)\|_*\leq rac{1}{\epsilon}\|y-x\|$$

Theorem

Lemma

$$\langle \nabla f(y_k), x_k - y_k \rangle \geq \frac{1}{4} \epsilon^{\frac{1}{p-1}} \| \nabla f(y_k) \|_*^{\frac{p}{p-1}}$$

Can use this to complete the modified discretization process!

Accelerated higher-order gradient method

$$\begin{aligned} x_{k+1} &= \frac{p}{k+p} z_k + \frac{k}{k+p} y_k \\ y_k &= \arg\min_{y} \left\{ f_{p-1}(y; x_k) + \frac{2}{\epsilon p} \|y - x_k\|^p \right\} &\leftarrow O\left(\frac{1}{\epsilon k^{p-1}}\right) \\ z_k &= \arg\min_{z} \left\{ Cpk^{(p-1)} \langle \nabla f(y_k), z \rangle + \frac{1}{\epsilon} D_h(z, z_{k-1}) \right\} \end{aligned}$$

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

$$f(y_k) - f(x^*) \leq O\left(rac{1}{\epsilon k^p}
ight) ~\leftarrow~$$
 accelerated rate

p = 2: Accelerated gradient/mirror descent

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

 $p \ge 2$: 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

$$O\left(\frac{1}{\epsilon k^{p-1}}\right) \text{ when } \nabla^{p-1}f \text{ is } \frac{1}{\epsilon}\text{-Lipschitz}$$
matching rate with $\epsilon = \delta^{p-1} \Leftrightarrow \delta = \epsilon^{\frac{1}{p-1}}$

Recap: Gradient vs. accelerated methods

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How to design dynamics for minimizing a convex function f?

Rescaled gradient flowPolynomial Euler-Lagrange equation
$$\dot{X}_t = -\nabla f(X_t) / \|\nabla f(X_t)\|_*^{\frac{p-2}{p-1}}$$
 $\mathcal{O}(\frac{1}{t^{p-1}})$ $\mathcal{O}\left(\frac{1}{t^{p-1}}\right)$ $\mathcal{O}\left(\frac{1}{t^p}\right)$ Higher-order gradient method $\mathcal{O}\left(\frac{1}{\epsilon k^{p-1}}\right)$ when $\nabla^{p-1}f$ is $\frac{1}{\epsilon}$ -Lipschitz $\mathcal{O}\left(\frac{1}{\epsilon k^p}\right)$ when $\nabla^{p-1}f$ is $\frac{1}{\epsilon}$ -Lipschitzmatching rate with $\epsilon = \delta^{p-1} \Leftrightarrow \delta = \epsilon^{\frac{1}{p-1}}$

Summary: Bregman Lagrangian

 Bregman Lagrangian family with general convergence guarantee

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

 Polynomial subfamily generates accelerated higher-order methods: O(1/t^p) convergence rate via higher-order smoothness

Summary: Bregman Lagrangian

 Bregman Lagrangian family with general convergence guarantee

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

- Polynomial subfamily generates accelerated higher-order methods: O(1/t^p) convergence rate via higher-order smoothness
- Exponential subfamily: $O(e^{-ct})$ rate via uniform convexity
- Understand structure and properties of Bregman Lagrangian: Gauge invariance, symmetry, gradient flows as limit points, etc.
- Bregman Hamiltonian:

$$\mathcal{H}(x,p,t) = e^{\alpha_t + \gamma_t} \left(D_{h^*} \left(\nabla h(x) + e^{-\gamma_t} p, \nabla h(x) \right) + e^{\beta_t} f(x) \right)$$

Discussion

- Many conceptual and mathematical challenges arising in taking seriously the problem of "Big Data"
- Facing these challenges will require a rapprochement between "computational thinking" and "inferential thinking"
 - bringing computational and inferential fields together at the level of their foundations