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
A Job Description, circa 2015

• Your Boss: “I need a Big Data system that will replace our classic service with a personalized service”
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• Your Boss: “I need a Big Data system that will replace our classic service with a personalized service”

• “It should work reasonably well for anyone and everyone; I can tolerate a few errors but not too many dumb ones that will embarrass us”
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• Your Boss: “I need a Big Data system that will replace our classic service with a personalized service”
• “It should work reasonably well for anyone and everyone; I can tolerate a few errors but not too many dumb ones that will embarrass us”
• “It should run just as fast as our classic service”
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• “It should only improve as we collect more data; in particular it shouldn’t slow down”
Your Boss: “I need a Big Data system that will replace our classic service with a personalized service”

“It should work reasonably well for anyone and everyone; I can tolerate a few errors but not too many dumb ones that will embarrass us”

“It should run just as fast as our classic service”

“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”
Some Challenges Driven by Big Data

- Big Data analysis requires a thorough blending of computational thinking and inferential 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.
Some Challenges Driven by Big Data

• 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 real-world 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 how 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

\[ \sim \theta \]

database
Privacy

query

\[ \text{database} \]

\[ \tilde{\theta} \]

\[ Q \]

query

\[ \text{privatized database} \]
Privacy

query → database → \tilde{\theta} → query

query → privatized database → \hat{\theta}
Classical problem in differential privacy: show that $\hat{\theta}$ and $\tilde{\theta}$ are close under constraints on $Q$. 
Inference

query

database

\hat{\theta}
Inference

\[ P \xrightarrow{S} \text{database} \]

query

\[ \tilde{\theta} \]
Inference

query

\[ P \]

\[ S \]

\[ \theta \]

\[ \tilde{\theta} \]
Classical problem in statistical theory: show that $\tilde{\theta}$ and $\theta$ are close under constraints on $S$
The privacy-meets-inference problem: show that $\theta$ 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 $\mathcal{P}$, a parameter $\theta(P)$ for each $P \in \mathcal{P}$, an estimator $\hat{\theta}$, and a loss $l(\hat{\theta}, \theta(P))$, define the risk:

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

$X_1 \rightarrow Z_1 \rightarrow \theta \rightarrow Z_n \rightarrow X_n$

$X_2 \rightarrow Z_2$

Private

Diagram showing the relationship between $X_1, X_2, \ldots, X_n$ and $Z_1, Z_2, \ldots, Z_n$ with arrows indicating the flow of information, and the variable $\theta$ at the center.
Local Privacy

Individuals $i \in \{1, \ldots, n\}$ with private data $X_i \overset{iid}{\sim} P$

Estimator $Z_1^n \rightarrow \hat{\theta}(Z_1^n)$
Definition: channel $Q$ is $\alpha$-differentially private if

$$\sup_{S,x\in X,x'\in X} \frac{Q(Z \in S \mid x)}{Q(Z \in S \mid x')} \leq \exp(\alpha)$$

[Dwork, McSherry, Nissim, Smith 06]

Given $Z$, cannot reliably discriminate between $x$ and $x'$
Private Minimax Risk

- Parameter $\theta(P)$ of distribution
- Family of distributions $\mathcal{P}$
- Loss $\ell$ measuring error
- Family $\mathcal{Q}_\alpha$ of private channels

$\alpha$-private Minimax risk

$$M_n(\theta(\mathcal{P}), \ell, \alpha) := \inf_{Q \in \mathcal{Q}_\alpha} \inf_{\hat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_{P,Q} \left[ \ell(\hat{\theta}(Z^n_1), \theta(P)) \right]$$

Best $\alpha$-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

<table>
<thead>
<tr>
<th>Substance</th>
<th>Proportion</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alcohol</td>
<td>0.45</td>
</tr>
<tr>
<td>Cocaine</td>
<td>0.32</td>
</tr>
<tr>
<td>Heroin</td>
<td>0.16</td>
</tr>
<tr>
<td>Cannabis</td>
<td>0.20</td>
</tr>
<tr>
<td>LSD</td>
<td>0.00</td>
</tr>
<tr>
<td>Amphetamines</td>
<td>0.02</td>
</tr>
</tbody>
</table>
Proposition:

Minimax rate

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

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

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

**Proposition:**

Private minimax rate for $\alpha = O(1)$

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

\[
\mathcal{M}_n(\mathcal{P}_d, \| \cdot \|_\infty, \alpha) \asymp \min \left\{ 1, \frac{\sqrt{d \log d}}{\sqrt{n\alpha^2}} \right\}
\]

**Note:** Effective sample size \( n \mapsto n\alpha^2/d \)
Optimal mechanism?

$X = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

$Z = X + W = \begin{bmatrix} 1 + W_1 \\ 0 + W_2 \\ 1 + W_3 \\ 0 + W_4 \\ 0 + W_5 \end{bmatrix}$

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

\[ X = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \]

Non-private observation
Optimal mechanism

\[
X = \begin{bmatrix}
1 \\
0 \\
1 \\
0 \\
0
\end{bmatrix} \quad v = \begin{bmatrix}
0 \\
1 \\
1 \\
0 \\
0
\end{bmatrix} \quad 1 - v = \begin{bmatrix}
1 \\
0 \\
0 \\
1 \\
1
\end{bmatrix}
\]

Non-private observation

View 1
(closer: 3 overlap)

• Draw \( \mathbf{v} \) uniformly in \( \{0, 1\}^d \)

View 2
(farther: 2 overlap)
Optimal mechanism

\[ X = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \]

Non-private observation

\[ v = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \]

View 1
(closer: 3 overlap)

\[ 1 - v = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \]

View 2
(farther: 2 overlap)

- Draw \( v \) uniformly in \( \{0, 1\}^d \)
- With probability \( \frac{e^\alpha}{1 + e^\alpha} \)
  choose closer of \( v \) and \( 1 - v \) to \( X \)
- otherwise, choose farther

At end:
Compute sample average and de-bias
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:

\[ n \mapsto \frac{n\alpha^2}{d} \]
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 \( m \) agents has sample of size \( n \)

\[ X^i = (X^i_1, X^i_2, \ldots, X^i_n) \]

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 $\theta(P)$ of distribution
- Family of distributions $\mathcal{P}$
- Loss $\|\cdot\|_2^2$

Constrained to be $\leq B$ bits
Minimax Communication

Central object of study:
- Parameter \( \theta(P) \) of distribution
- Family of distributions \( \mathcal{P} \)
- Loss \( \| \cdot \|_2^2 \)

Constrained to be \( \leq B \) bits

Minimax risk with \( B \)-bounded communication

\[
\mathcal{M}_n(\theta(\mathcal{P}), B) := \inf_{\pi \in \Pi_B} \inf_{\hat{\theta}} \sup_{P \in \mathcal{P}} \mathbb{E}_P \left[ \| \hat{\theta}(Z_1^m) - \theta(P) \|_2^2 \right]
\]

Best protocol \( Z_i = \pi(X^i) \) with \( Z_i \) smaller than \( B \) bits
Consider estimation in normal location family, $\theta \in [-1, 1]^d$

$$X^i_j \overset{iid}{\sim} \mathcal{N}(\theta, \sigma^2 I_{d \times d})$$
Vignette: Mean Estimation

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

\[
X^i_j \overset{i.i.d.}{\sim} N(\theta, \sigma^2 I_{d \times d})
\]

**Theorem:** when each agent has sample of size \( n \)

Minimax rate

\[
\mathbb{E}[\|\hat{\theta}(X^1, \ldots, X^m) - \theta\|_2^2] \asymp \frac{\sigma^2 d}{nm}
\]
Vignette: Mean Estimation

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

$$X_j^i \overset{iid}{\sim} \mathcal{N}(\theta, \sigma^2 I_{d \times d})$$

**Theorem:** when each agent has sample of size $n$

Minimax rate with $B$-bounded communication

$$\frac{d}{B \wedge d \log m} \cdot \frac{1}{nm} \cdot \frac{\sigma^2 d}{\leq \mathcal{M}_n(N_d, B) \leq \frac{d \log m}{B \wedge d} \cdot \frac{\sigma^2 d}{nm}}$$
Vignette: Mean Estimation

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

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

**Theorem:** when each agent has sample of size $n$

Minimax rate with $B$-bounded communication

$$\frac{d}{B \wedge d \log m} \frac{1}{nm} \leq \mathcal{M}_n(N_d, B) \leq \frac{d \log m}{B \wedge d} \frac{\sigma^2 d}{nm}$$

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

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

**Setting:** Unconstrained convex optimization

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\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:
  \[
  y_{k+1} = x_k - \beta \nabla f(x_k)
  \]
  \[
  x_{k+1} = (1 - \lambda_k)y_{k+1} + \lambda_k y_k
  \]
  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
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

- Analysis using Nesterov’s estimate sequence technique
- Common interpretation as “momentum methods” (Euclidean case)

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

- Analysis using Nesterov’s estimate sequence technique
- 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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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)
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)

- Su, Boyd, Candes '14: Continuous time limit of accelerated gradient descent is a second-order ODE
  \[ \ddot{X}_t + \frac{3}{t} \dot{X}_t + \nabla f(X_t) = 0 \]
Accelerated methods: Continuous time perspective

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  (and mirror descent is discretization of natural gradient flow)

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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**:

\[ \mathcal{L}(x, \dot{x}, t) = e^{\gamma t + \alpha t} \left( D_h(x + e^{-\alpha t} \dot{x}, x) - e^{\beta t} f(x) \right) \]
Bregman Lagrangian

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- Function of position \( x \), velocity \( \dot{x} \), and time \( t \)
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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**
**Bregman Lagrangian**

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- \(f\) is the convex objective function

![Diagram](image.png)
Bregman Lagrangian

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  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

Ideal scaling conditions:

\[ \dot{\beta}_t \leq e^{\alpha t} \dot{\gamma}_t = e^{\alpha t} \]

Diagram:

- \( h(y) \)
- \( D_h(y, x) \)
- \( h(x) \)
- \( x \rightarrow y \)
- \( x \)
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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\[ \dot{\beta}_t \leq e^{\alpha t} \]
\[ \dot{\gamma}_t = e^{\alpha t} \]
Bregman Lagrangian

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Variational problem over curves:

\[ \min_{\chi} \int \mathcal{L}(X_t, \dot{X}_t, t) \, dt \]

Optimal curve is characterized by Euler-Lagrange equation:

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

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

E-L equation for Bregman Lagrangian under ideal scaling:

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

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

\[ f(X_t) - f(x^*) \leq O(e^{-\beta t}) \]
General convergence rate

**Theorem**

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

\[ f(X_t) - f(x^*) \leq O(e^{-\beta t}) \]

**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)

\((p = 2: \text{accelerated gradient descent})\)

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

\[ \text{speed up time: } Y_t = X_{t^{3/2}} \]

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

\((p = 3: \text{accelerated cubic-regularized Newton’s method})\)
Time dilation property (reparameterizing time)

\[(p = 2: \text{accelerated gradient descent})\]

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

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\[(p = 3: \text{accelerated cubic-regularized Newton’s method})\]

- 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

\[ O(e^{-\beta t}) : \text{E-L for Lagrangian } \mathcal{L}_{\alpha, \beta, \gamma} \]

\[ \text{speed up time: } Y_t = X_{\tau(t)} \]

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

where

\[ \tilde{\alpha}_t = \alpha_{\tau(t)} + \log \dot{\tau}(t) \]

\[ \tilde{\beta}_t = \beta_{\tau(t)} \]

\[ \tilde{\gamma}_t = \gamma_{\tau(t)} \]
Time dilation for general Bregman Lagrangian

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\[ \tilde{\gamma}_t = \gamma_{\tau(t)} \]

**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:

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

\[ \frac{d}{dt} \nabla h(Z_t) = -Cpt^{p-1} \nabla f(X_t) \]
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 $x_k = X_t$, $x_{k+1} = X_{t+\delta}$):

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

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

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

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

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
Modified discretization

Introduce an auxiliary sequence $y_k$:

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

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

How?

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

Theorem

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

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Proof using generalization of Nesterov's estimate sequence technique
Higher-order gradient update

Higher-order Taylor approximation of $f$:

$$ f_{p-1}(y; x) = f(x) + \langle \nabla f(x), y - x \rangle + \cdots + \frac{1}{(p-1)!} \nabla^{p-1} f(x)(y - x)^{p-1} $$

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 $f$:

$$f_{p-1}(y; x) = f(x) + \langle \nabla f(x), y - x \rangle + \cdots + \frac{1}{(p-1)!} \nabla^{p-1}f(x)(y - x)^{p-1}$$

Higher-order gradient update:

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

Assume $f$ is smooth of order $p - 1$:

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

Theorem

Lemma

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

Can use this to complete the modified discretization process!
Accelerated higher-order gradient method

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

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

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

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

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

\( p = 2 \): 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

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

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

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 $\epsilon = \delta^{p-1} \iff \delta = \epsilon^{1/p-1}$
Recap: Gradient vs. accelerated methods

How to design dynamics for minimizing a convex function $f$?

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<td>$\dot{X}_t = -\nabla f(X_t) / |\nabla f(X_t)|^{p-2}$</td>
<td>$\ddot{X}_t + \frac{p+1}{t} \dot{X}_t + t^{p-2} \left[\nabla^2 h\left(X_t + \frac{t}{p} \dot{X}_t\right)\right]^{-1} \nabla f(X_t) = O\left(\frac{1}{t^p}\right)$</td>
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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