Robust empirical risk minimization via Newton’s method

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CRiSM Seminar
University of Warwick

11 January 2023

Joint work with Eirini Ioannou (Edinburgh) and Muni Sreenivas Pydi (Université Paris Dauphine)
Goal: Parametric estimation in contaminated data

Huber’s $\epsilon$-contamination model: Observations $z_i \sim (1 - \epsilon)\mathcal{P}_{\theta^*} + \epsilon Q$, where $Q$ is arbitrary
Introduction

- **Goal:** Parametric estimation in contaminated data
- Huber’s $\epsilon$-contamination model: Observations $z_i \sim (1 - \epsilon)P_{\theta^*} + \epsilon Q$, where $Q$ is arbitrary
- Our method is also applied to heavy-tailed parametric estimation (no contamination)
Traditional approach via $M$-estimators: Suppose

$$
\theta^* = \arg \min_{\theta} \mathbb{E}_{x_i \sim P_{\theta^*}} [\mathcal{L}(\theta, x_i)]
$$

Use empirical risk minimizer

$$
\hat{\theta} \in \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(\theta, z_i),
$$

for appropriately defined $\mathcal{L}$
● Alternative approach: Use “non-robust” $\mathcal{L}$ (e.g., based on log-likelihood of $P_\theta$) and robustify optimization procedure
Robust gradient descent algorithm (Prasad, Suggala, Balakrishnan, and Ravikumar (2020)):

\[ \theta_{t+1} = \theta_t - \eta g(\theta_t), \]

where \( g(\theta_t) \) is an estimate of \( \nabla R(\theta_t) \).
Previous work

- SEVER algorithm (Diakonikolas, Kamath, Kane, Li, Steinhardt, and Stewart (2019)) uses an “approximate learner” algorithm which finds approximately critical points.

- Iteratively filters out data points with outlying gradients computed at $\theta_t$, chosen by the approximate learner.
Previous work

- Median-of-means minimization approach (Lecué, Lerasle, and Mathieu (2020)) performs gradient descent by computing gradients w.r.t. a median block (computed w.r.t. empirical mean of $\mathcal{L}$) on each iterate.
- Derives excess risk bounds on final iterate.
We analyze a second-order version of Prasad et al. (2020), based on Newton’s method:

\[ \theta_{t+1} = \theta_t - \alpha_t H(\theta_t)^{-1} g(\theta_t), \]

where \((g(\theta_t), H(\theta_t))\) are estimates of \((\nabla R(\theta_t), \nabla^2 R(\theta_t))\) and \(\alpha_t\) is a step size.
We analyze a second-order version of Prasad et al. (2020), based on Newton’s method:

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where \((g(\theta_t), H(\theta_t))\) are estimates of \((\nabla R(\theta_t), \nabla^2 R(\theta_t))\) and \(\alpha_t\) is a step size.

Benefit of second-order algorithm: faster convergence to optimum (quadratic rather than linear convergence)
Robust estimators: Huber contamination

- Algorithm of Lai, Rao, and Vempala (2016) for multivariate mean estimation

```
Algorithm 3: AGNOSTICMEAN(S)

Input: $S \subset \mathbb{R}^n$, and a routine OUTLIERRemoval().
Output: $\hat{\mu} \in \mathbb{R}^n$.

1. Let $(\tilde{S}, w) = \text{OUTLIERRemoval}(S)$.
2. if $n = 1$:
   (a) if $w = -1$, Return median($\tilde{S}$). //Gaussian case
   (b) else Return mean($\tilde{S}$). //General case
3. Let $\Sigma_{\tilde{S},w}$ be the weighted covariance matrix of $\tilde{S}$ with weights $w$, and $V$ be the span of the top $n/2$ principal components of $\Sigma_{\tilde{S},w}$, and $W$ be its complement.
4. Set $S_1 := P_V(S)$ where $P_V$ is the projection operation on to $V$.
5. Let $\hat{\mu}_V := \text{AGNOSTICMEAN}(S_1)$ and $\hat{\mu}_W := \text{mean}(P_W\tilde{S})$.
6. Let $\hat{\mu} \in \mathbb{R}^n$ be such that $P_V\hat{\mu} = \hat{\mu}_V$ and $P_W\hat{\mu} = \hat{\mu}_W$.
7. Return $\hat{\mu}$.
```
Robust estimators: Huber contamination

For gradients, we treat vectors \( \{\nabla \mathcal{L}(\theta, z_i)\}_{i=1}^n \) as contaminated samples from a distribution with mean \( \nabla \mathcal{R}(\theta) \in \mathbb{R}^p \).

For Hessians, we vectorize matrices \( \{\nabla^2 \mathcal{L}(\theta, z_i)\}_{i=1}^n \) and treat them as contaminated samples from a distribution with mean \( \nabla^2 \mathcal{R}(\theta) \in \mathbb{R}^{p \times p} \).
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Traditional Newton’s method analysis (e.g., Boyd and Vandenberghe (2004)) involves picking step size $\alpha_t$ using a linesearch algorithm.
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Robust version involves a slightly modified version of loss function evaluation and introduction of error parameter:

Set $\alpha = 1$

While $\text{RobustEstimate} \left( \{ \mathcal{L}(\theta + \alpha \Delta \theta_{nt}, z_i) \}_{i=1}^{n} \right) > \text{RobustEstimate} \left( \{ \mathcal{L}(\theta, z_i) \}_{i=1}^{n} \right) + \kappa_1 \alpha g(\theta) \Delta \theta_{nt} + \zeta$ do

Update $\alpha = \kappa_2 \alpha$

End while
Backtracking linesearch

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- Robust version involves a slightly modified version of loss function evaluation and introduction of error parameter:
  
  Set $\alpha = 1$
  
  while $\text{RobustEstimate}(\{L(\theta + \alpha \Delta \theta_{nt}, z_i)\}_{i=1}^{n}) > \text{RobustEstimate}(\{L(\theta, z_i)\}_{i=1}^{n}) + \kappa_1 \alpha g(\theta) \Delta \theta_{nt} + \zeta$ do
  
  Update $\alpha = \kappa_2 \alpha$

end while

- Newton direction is $\Delta \theta_{nt} := -H(\theta_t)^{-1}g(\theta_t)$, contraction parameter is $\kappa_2 \in (0, 1)$, and step size is output of backtracking algorithm.
Convergence guarantees

- Assume population-level objective satisfies strong convexity/smoothness:
  \[ mI \preceq \nabla^2 R(\theta) \preceq MI \]
  (in a local region around \( \theta^* \))

- Also assume \( \nabla^2 R \) is \( L \)-Lipschitz
Convergence guarantees

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- In traditional Newton’s method analysis, iterates decrease objective by constant increments during damped Newton phase, then exhibit fast convergence with step size \( \alpha_t = 1 \) (pure Newton phase)
Convergence guarantees

Assume gradient/Hessian errors are small:

\[ \| g(\theta_t) - \nabla R(\theta_t) \|_2 \leq \alpha_g \| \theta_t - \theta^* \|_2 + \beta_g, \]
\[ \| H(\theta_t) - \nabla^2 R(\theta_t) \|_2 \leq \alpha_h \| \theta_t - \theta^* \|_2 + \beta_h, \]

for all \( 1 \leq t \leq T \)
Convergence guarantees

- Assume gradient/Hessian errors are small:
  
  \[
  \|g(\theta_t) - \nabla \mathcal{R}(\theta_t)\|_2 \leq \alpha_g \|\theta_t - \theta^*\|_2 + \beta_g, \\
  \|H(\theta_t) - \nabla^2 \mathcal{R}(\theta_t)\|_2 \leq \alpha_h \|\theta_t - \theta^*\|_2 + \beta_h,
  \]
  
  for all \(1 \leq t \leq T\)

- Also assume robust loss estimates are smaller than \(\frac{\zeta}{4}\) for all evaluations of backtracking linesearch
Convergence guarantees

Theorem (Pure Newton phase)

Suppose $\|\nabla R(\theta_0)\|_2 < \eta(m, L)$. Then backtracking linesearch chooses $\alpha_t = 1$ on all successive iterates, and $\|\nabla R(\theta_t)\|_2 < \eta$ and

$$\|\theta_t - \theta^*\|_2 \leq \frac{m}{L} \left(\frac{1}{2}\right)^{2^t} + c(m, L) \bigg( O(\alpha_g + \beta_g + \alpha_h + \beta_h) \bigg),$$

for all $1 \leq t \leq T$. 
Convergence guarantees

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$$\| \theta_t - \theta^* \|_2 \leq \frac{m}{L} \left( \frac{1}{2} \right)^{2t} + c(m, L) \underbrace{O(\alpha_g + \beta_g + \alpha_h + \beta_h)}_{\omega},$$

for all $1 \leq t \leq T$.

- For Huber contamination, parameters $(\alpha_g, \beta_g, \alpha_h, \beta_h)$ will be functions of $\epsilon$ (e.g., all are $O(\sqrt{\epsilon})$ in GLMs)
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- For Huber contamination, parameters $(\alpha_g, \beta_g, \alpha_h, \beta_h)$ will be functions of $\epsilon$ (e.g., all are $O(\sqrt{\epsilon})$ in GLMs).
- Proper choice of $\zeta$ is also $O(\alpha_g + \beta_g + \alpha_h + \beta_h)$.
- After $\log \log \left(\frac{1}{\omega}\right)$ iterations (as opposed to $\log \left(\frac{1}{\omega}\right)$, for robust gradient descent), error becomes $O(\omega)$. 

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Convergence guarantees

Theorem (Damped Newton phase)

Suppose $\|\nabla R(\theta_t)\|_2 \geq \eta(m, L)$. There exists some $\gamma(m, M, L) > 0$ such that after a constant number of function evaluations, backtracking linesearch chooses a step size such that

$$R(\theta_{t+1}) - R(\theta_t) < -\gamma(m, M, L).$$
Convergence guarantees

**Theorem (Damped Newton phase)**

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$$R(\theta_{t+1}) - R(\theta_t) < -\gamma(m, M, L).$$

- Thus, number of iterates in damped Newton phase is upper-bounded
Proof elements

- At some level, “just add some error terms to usual Newton analysis”
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- Although linesearch exit condition is

$$R(\theta_t + \alpha \Delta \theta_t) \leq R(\theta_t) - \kappa \alpha \lambda^2(\theta_t) + \zeta,$$

  can show lower bound on step size, leading to sufficient decrease
Proof elements

- At some level, “just add some error terms to usual Newton analysis”
- In pure Newton phase, need to show backtracking linesearch still only chooses $\alpha_t = 1$
- In damped Newton phase, show backtracking linesearch still chooses descent directions (in fact, $R(\theta_{t+1}) - R(\theta_t) < -\gamma$)
- Although linesearch exit condition is
  \[
  R(\theta_t + \alpha \Delta \theta_t) \leq R(\theta_t) - \kappa \alpha \lambda^2(\theta_t) + \zeta,
  \]
  can show lower bound on step size, leading to sufficient decrease
- Also need to show that iterates lie in a ball around $\theta^*$, in order to obtain uniform upper bound on gradient/Hessian errors:
  \[
  \|\theta_t - \theta^*\|_2 \leq \gamma_0
  \]
Heavy-tailed distributions

- Can use same Newton’s method framework to obtain parameter estimates for heavy-tailed data

```markdown

Require:
- Samples $S = \{s_i\}_{n_i=1}^n$
- Failure probability $\delta$

1: function HeavyTailedEstimator($S = \{s_i\}_{n_i=1}^n$, $\delta$)

2: Set $b = 1 + \lceil 3.5 \log \frac{1}{\delta} \rceil$, the number of buckets.

3: Partition $S$ into $b$ blocks $B_1, \ldots, B_b$, each of size $\lceil n/b \rceil$.

4: for $i = 1, \ldots, n$

5: \hat{\mu}_i = \frac{1}{|B_i|} \sum_{s \in B_i} s$

6: end for

7: Set $\hat{\mu} = \arg \min_b \sum_{i=1}^n \| \mu - \hat{\mu}_i \|_2$

8: return $\hat{\mu}$.
```
Heavy-tailed distributions

- Can use same Newton’s method framework to obtain parameter estimates for heavy-tailed data

**Require:** Samples $S = \{s_i\}_{i=1}^n$, Failure probability $\delta$

1. **function** HEAVYTailedESTIMATOR($S = \{s_i\}_{i=1}^n$, $\delta$)
   2. Set $b = 1 + \lceil 3.5 \log 1/\delta \rceil$, the number of buckets.
   3. Partition $S$ into $b$ blocks $B_1, \ldots, B_b$, each of size $\lfloor n/b \rfloor$.
   4. **for** $i = 1 \ldots n$ **do**
      5. $\hat{\mu}_i = \frac{1}{|B_i|} \sum_{s \in B_i} s$.
   6. **end** **for**
   7. Set $\hat{\mu} = \arg \min_{\mu} \sum_{i=1}^b \| \mu - \hat{\mu}_i \|_2$. 
      
      return $\hat{\mu}$.
   8. **end function**
Application to GLMs

Assume

$$P_{\theta^*}(y|x) \propto \exp \left( \frac{y x^T \theta^* - \Phi(x^T \theta^*)}{c(\sigma)} \right),$$

where $\Phi$ is the link function and

$$\mathcal{L}(\theta, (x_i, y_i)) = -y x^T \theta + \Phi(x^T \theta)$$

is the negative log-likelihood.
Application to GLMs

- Assume

\[ P_{\theta^*}(y|x) \propto \exp \left( \frac{yx^T \theta^* - \Phi(x^T \theta^*)}{c(\sigma)} \right), \]

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- Assume regularity conditions on \( \Phi \) (bounded derivatives and moments of derivatives)
Application to GLMs

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is the negative log-likelihood

- Assume regularity conditions on \( \Phi \) (bounded derivatives and moments of derivatives)

- Assume bounded eighth moments of \( x_i \)'s
Suppose \( \{z_i\}_{i=1}^n \) are i.i.d. draws from a Huber \( \epsilon \)-contaminated GLM.

Suppose \( n = \Omega \left( p + \epsilon p^2 + \frac{1}{\sqrt{\delta}} \right) \). Then the robust Newton method with \( T \asymp \log \log \left( \frac{1}{\epsilon} \right) \) returns an output satisfying

\[
\| \theta_T - \theta^* \|_2 = O \left( p^2 \sqrt{\epsilon \log p} \right),
\]

with probability at least \( 1 - T' \delta \).
Application to GLMs

**Theorem (Huber contamination)**

Suppose \( \{z_i\}_{i=1}^n \) are i.i.d. draws from a Huber \( \epsilon \)-contaminated GLM. Suppose \( n = \Omega \left( p + \epsilon p^2 + \frac{1}{\sqrt{\delta}} \right) \). Then the robust Newton method with \( T \asymp \log \log \left( \frac{1}{\epsilon} \right) \) returns an output satisfying

\[
\| \theta_T - \theta^* \|_2 = O \left( p^2 \sqrt{\epsilon \log p} \right),
\]

with probability at least \( 1 - T' \delta \)

- Under additional assumptions on the covariates (e.g., 4-wise independence of coordinates), estimation error can be reduced to \( O(\sqrt{\epsilon \log p}) \)
In order to apply earlier theorem, need to determine \((\alpha_g, \beta_g, \alpha_h, \beta_h)\).

Analysis of Lai et al. (2016) shows

\[
\|g(\theta) - \nabla R(\theta)\|_2 = O \left( \sqrt{\|\text{Cov}(\nabla R(\theta))\|_2} \epsilon \log p \right)
\]

Thus, we need bounds on \(\|\text{Cov}(\nabla R(\theta))\|_2\) (and similarly, on \(\|\text{Cov}(\text{flatten}(\nabla^2 R(\theta)))\|_2\))
Theorem (Heavy-tailed distributions)

Suppose \( \{z_i\}_{i=1}^n \) are i.i.d. draws from a heavy-tailed distribution. Suppose \( n = \Omega \left( p^2 \log \left( \frac{1}{\delta} \right) \right) \). Then the robust Newton method with

\[
T \asymp \log \log \left( \frac{n}{p^2} \right)
\]

returns an output satisfying

\[
\| \theta_T - \theta^* \|_2 = O \left( \sqrt{\frac{p^2}{n}} \right),
\]

with probability at least \( 1 - T' \delta \).
Suppose \( \{ z_i \}_{i=1}^n \) are i.i.d. draws from a heavy-tailed distribution. Suppose \( n = \Omega \left( p^2 \log \left( \frac{1}{\delta} \right) \right) \). Then the robust Newton method with
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with probability at least \( 1 - T' \delta \)

- Again, assuming 4-wise independence of coordinates of the covariates, we can tighten the error bound to \( O \left( \sqrt{\frac{p}{n}} \right) \)
Application to GLMs

Theorem (Heavy-tailed distributions)

Suppose \( \{z_i\}_{i=1}^n \) are i.i.d. draws from a heavy-tailed distribution. Suppose \( n = \Omega \left( p^2 \log \left( \frac{1}{\delta} \right) \right) \). Then the robust Newton method with \( T \asymp \log \log \left( \frac{n}{p^2} \right) \) returns an output satisfying

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\| \theta_T - \theta^* \|_2 = O \left( \sqrt{\frac{p^2}{n}} \right)
\]

with probability at least \( 1 - T'\delta \)

- Again, assuming 4-wise independence of coordinates of the covariates, we can tighten the error bound to \( O \left( \sqrt{\frac{p}{n}} \right) \)
- Here, we can show that \( \alpha_g, \beta_g, \alpha_h, \beta_h = O \left( \frac{p^2 \log(1/\delta)}{n} \right) \)
Conjugate gradient method

- Alternative version of robust Newton’s method, inspired by Martens (2010), approximates Hessian-vector products via finite differences:

\[ \nabla^2 f(\theta)v \approx \frac{\nabla f(\theta + \delta v) - \nabla f(\theta)}{\delta} \]
Conjugate gradient method

- Alternative version of robust Newton’s method, inspired by Martens (2010), approximates Hessian-vector products via finite differences:

\[
\nabla^2 f(\theta) v \approx \frac{\nabla f(\theta + \delta v) - \nabla f(\theta)}{\delta}
\]

- Newton direction \( \Delta \theta_t \) (for population-level objective) satisfies

\[
\nabla^2 \mathcal{R}(\theta_t) \Delta \theta_t = -\nabla \mathcal{R}(\theta_t)
\]
Conjugate gradient method

- Conjugate gradient algorithm (Wright & Nocedal (1999)) provides iterative method for solving linear system $Ax = b$, where only products of the form $Av$ are required for updates

\[
\begin{align*}
\text{Set } r_0 &= h_{\Delta \theta(0)}(\theta) + g(\theta) \\
\text{Set } p_0 &= -r_0 \\
\text{for } k = 1 \text{ to } p - 1 \text{ do} \\
&\quad \text{Compute Hessian-vector product estimate, } \quad h_{p_k}(\theta) = \text{HVPRODUCT}(\theta, p_k) \\
&\quad \text{Set } \alpha_k = \frac{r_k^T r_k}{p_k^T h_{p_k}(\theta)} \\
&\quad \text{Set } \Delta \theta^{(k+1)} = \Delta \theta^{(k)} + \alpha_k p_k \\
&\quad \text{Set } r_{k+1} = r_k + \alpha_k h_{p_k}(\theta) \\
&\quad \text{Set } \beta_{k+1} = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k} \\
&\quad \text{Set } p_{k+1} = -r_{k+1} + \beta_{k+1} p_k \\
\text{end for}
\]
Our idea: Run conjugate gradient algorithm to obtain approximate Newton steps, so only robust gradient vector evaluations are required.
Conjugate gradient method

- Our idea: Run conjugate gradient algorithm to obtain approximate Newton steps, so only robust \textit{gradient vector} evaluations are required
- (In practice, also need to choose parameter $\delta > 0$ for finite difference calculations)
Preceding analysis of robust Newton’s method only requires that Newton directions satisfy

$$\nabla \mathcal{R}(\theta_t) = -\nabla^2 \mathcal{R}(\theta_t) \Delta \theta_t + \chi_t,$$

where $\chi_t$ is a small, bounded error.
Conjugate gradient method: Theory?

- Preceding analysis of robust Newton’s method only requires that Newton directions satisfy

\[ \nabla R(\theta_t) = -\nabla^2 R(\theta_t) \Delta \theta_t + \chi_t, \]

where \( \chi_t \) is a small, bounded error.

- We can also think of conjugate gradient method as providing a direction that satisfies this approximate equation.
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However, we need to quantify propagation of errors through conjugate gradient iterates, due to robust estimators/finite difference approximation.
Preceding analysis of robust Newton’s method only requires that Newton directions satisfy
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We can also think of conjugate gradient method as providing a direction that satisfies this approximate equation.

However, we need to quantify propagation of errors through conjugate gradient iterates, due to robust estimators/finite difference approximation.

This seems to be an open question in optimization . . .
Conjecture: Approximate conjugate gradient method may converge geometrically to a small ball around true solution to linear system: If $A x^* = b$, then

$$\|x_s - x^*\|_A \leq 2\kappa^s \|x_0 - x^*\|_A + \text{err}$$
Conjecture: Approximate conjugate gradient method may converge geometrically to a small ball around true solution to linear system: If $Ax^* = b$, then

$$\|x_s - x^*\|_A \leq 2\kappa^s\|x_0 - x^*\|_A + \text{err}$$

Taylor expansion implies optimal choice of $\delta$ would be $C\epsilon^{1/4}$, leading to overall error rate of $O(\epsilon^{1/4})$ (possibly more widely applicable than the robust Newton method, which gives $O(\epsilon^{1/2})$ error rate in analyzable settings, e.g., GLMs)
Contributions

- Established framework of analysis for robust second-order optimization algorithm for parameter estimation
- Noisy analysis of backtracking linesearch succeeds in finding approximate Newton directions
- Proposed alternative robust Newton method based on conjugate gradient method
Open questions

- Better robust matrix estimators
- High-dimensional extensions
- Theory for conjugate gradient version
- Inexact Newton methods

Thank you!!