Stochastic Second-Order Optimization Methods Part II: Non-Convex

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Non-Convex Is Hard!

• Saddle points, Local Minima, Local Maxima



• 2nd Order Necessary Condition

$$\nabla F(\mathbf{x}^{\star}) = 0 \qquad \nabla^2 F(\mathbf{x}^{\star}) \succeq 0$$

• 2nd Order Sufficient Condition

$$\nabla F(\mathbf{x}^{\star}) = 0 \qquad \nabla^2 F(\mathbf{x}^{\star}) \succ 0$$

Non-Convex Is Hard!

- Additional complexity issues...
 - Optimization of a degree four polynomial: NP-hard [Hillar et al., 2013]
 - Checking for sufficient optimality condition: co-NP-complete [Murty et al., 1987]
 - Checking whether a point is not a local minimum: NP-complete [Murty et al., 1987]

All convex problems are the same, while every non-convex problem is different.

Not sure who's quote this is!

 $(\epsilon_{g}, \epsilon_{H}) - Optimality$

$\| abla F(\mathbf{x})\| \leq \epsilon_{\mathbf{g}}$ and $\lambda_{\min}(abla^2 F(\mathbf{x})) \geq -\epsilon_{\mathbf{H}}$

Outline

- Part I: Convex
 - Smooth
 - Newton-CG
 - Non-Smooth
 - Proximal Newton
 - Semi-smooth Newton
- Part II: Non-Convex
 - Line-Search Based Methods
 - L-BFGS
 - Gauss-Newton
 - Natural Gradient
 - Trust-Region Based Methods
 - Trust-Region
 - Cubic Regularization
- Part III: Discussion and Examples

- Sad Note 🙂: BFGS may fail on non-convex problems with both exact line search [Mascarenhas, 2004] and inexact (e.g., Wolfe) variants [Dai, 2002]
- Happy Note 🙂: BFGS dominates in many practical non-convex applications

Newton's Method: Scalar Case

Finding a root of $r: \mathbb{R} \to \mathbb{R}$, i.e., find x^* for which $r(x^*) = 0$:

$$0 = r(x^{*}) = r(x^{(k)}) + (x^{*} - x^{(k)}) r'(x^{(k)}) + o(|x^{*} - x^{(k)}|)$$

$$0 = r(x^{(k)}) + \left(x^{(k+1)} - x^{(k)}\right)r'(x^{(k)})$$

$$x^{(k+1)} = x^{(k)} - \frac{r(x^{(k)})}{r'(x^{(k)})}.$$

Secant Method: Scalar Case

Finding a root of $r : \mathbb{R} \to \mathbb{R}$, i.e., find x^* for which $r(x^*) = 0$:

Approximate the derivative: $r'(x^{(k)}) \approx \frac{r(x^{(k)}) - r(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$

$$x^{(k+1)} = x^{(k)} - \left(\frac{x^{(k)} - x^{(k-1)}}{r(x^{(k)}) - r(x^{(k-1)})}\right) r(x^{(k)}).$$

Local convergence rate is

$$\left|x^{(k+1)} - x^{\star}\right| \leq C \left|x^{(k)} - x^{\star}\right| \stackrel{\text{"Golden Ratio"}}{\underbrace{\frac{1 + \sqrt{5}}{2}}}$$

In contrast, rate of convergence of Newton is quadratic!

Quasi-Newton Method

Quasi-Newton optimization methods extend secant method to multivariable case!

Quasi-Newton Method

For
$$r(x) = f'(x)$$
, we have
$$f''(x^{(k)}) \approx \frac{f'(x^{(k)}) - f'(x^{(k-1)})}{x^{(k)} - x^{(k-1)}},$$
 i.e.,

$$f''(x^{(k)})\left(x^{(k)}-x^{(k-1)}\right) \approx f'(x^{(k)})-f'(x^{(k-1)}).$$

Quasi-Newton Method

$$\nabla f(\mathbf{x} + \mathbf{p}) = \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})\mathbf{p} + \int_0^1 \left[\nabla^2 f(\mathbf{x} + t\mathbf{p}) - \nabla^2 f(\mathbf{x})\right] \mathbf{p} \, \mathrm{d}t$$
$$= \nabla f(\mathbf{x}) + \nabla^2 f(\mathbf{x})\mathbf{p} + o(\|\mathbf{p}\|),$$
i.e., when $\mathbf{x} = \mathbf{x}^{(k)}, \mathbf{p} = \mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}$, and $\|\mathbf{p}\| \ll 1$, we have
$$\nabla^2 f(\mathbf{x}) = \mathbf{x}^{(k-1)} - \mathbf{x}^{(k)}, \quad \forall \mathbf{p} \in \mathcal{F}(\mathbf{x})$$

$$\nabla^2 f(\mathbf{x}^{(k)}) \left(\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)} \right) \approx \left(\nabla f(\mathbf{x}^{(k)}) - \nabla f(\mathbf{x}^{(k-1)}) \right)$$

Quasi-Newton Method

$$\nabla^2 f(\mathbf{x}^{(k)}) \left(\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)} \right) \approx \left(\nabla f(\mathbf{x}^{(k)}) - \nabla f(\mathbf{x}^{(k-1)}) \right)$$

So, look for $\mathbf{H}^{(k)} \approx \nabla^2 f(\mathbf{x}^{(k)})$ such that

$$\underbrace{\mathbf{H}^{(k)}\left(\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\right) = \left(\nabla f(\mathbf{x}^{(k)}) - \nabla f(\mathbf{x}^{(k-1)})\right)}_{\text{Secant Condition}}$$

Quasi-Newton Method: Another Interpretation

Another interpretation of the secant condition...

Quasi-Newton Method: Another Interpretation

Recall:

Iterative Scheme

$$\mathbf{y}^{(k)} = \underset{\mathbf{x}\in\mathcal{X}}{\operatorname{argmin}} \left\{ (\mathbf{x} - \mathbf{x}^{(k)})^T \mathbf{g}^{(k)} + \frac{1}{2} (\mathbf{x} - \mathbf{x}^{(k)})^T \mathbf{H}^{(k)} (\mathbf{x} - \mathbf{x}^{(k)}) \right\}$$
$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \left(\mathbf{y}^{(k)} - \mathbf{x}^{(k)} \right)$$

Quasi-Newton Method: Another Interpretation

- Suppose we have a $\mathbf{H}^{(k)}$ and $\mathbf{x}^{(k+1)}$
- How to update H^(k) to obtain a <u>new</u> quadratic approximation to F(x) at x^(k+1)?

$$m_{k+1}(\mathbf{p}) \triangleq f(\mathbf{x}^{(k+1)}) + \left\langle \nabla f(\mathbf{x}^{(k+1)}), \mathbf{p} \right\rangle + \frac{1}{2} \left\langle \mathbf{p}, \mathbf{H}^{(k+1)} \mathbf{p} \right\rangle$$

One reasonable requirement, suggested by Davidon, is

- $\nabla m_{k+1}(\mathbf{0}) = \nabla f(\mathbf{x}^{(k+1)}) \longrightarrow$ trivially satisfied
- $\nabla m_{k+1}(-\alpha \mathbf{p}_k) = \nabla f(\mathbf{x}^{(k)}) \longrightarrow \text{secant condition}$

Quasi-Newton Method: DFP

The revolution began with...



William C. Davidon

DFP: Davidon-Fletcher-Powell scheme

Quasi-Newton Method

$$\mathbf{H}^{(k)}\left(\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\right) = \left(\nabla f(\mathbf{x}^{(k)})-\nabla f(\mathbf{x}^{(k-1)})\right).$$

d equations vs. d^2 unknowns

The difference between QNMs boils down to how they update $\mathbf{H}^{(k)}$ (or its inverse)!

Quasi-Newton Method

Typical notation in QN literature:

$$\begin{aligned} \mathbf{s}_k &\triangleq \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} \\ \mathbf{y}_k &\triangleq \nabla f(\mathbf{x}^{(k+1)}) - \nabla f(\mathbf{x}^{(k)}) \end{aligned}$$

Quasi-Newton Method: BFGS

Updating
$$\mathbf{B}^{(k)} \triangleq \left[\mathbf{H}^{(k)}\right]^{-1}$$
:

$$\min_{\mathbf{B} \in \mathbb{R}^{d \times d}} \|\mathbf{B} - \mathbf{B}^{(k)}\|$$
s.t. $\mathbf{B} = \mathbf{B}^{T}$, $\mathbf{s}_{k} = \mathbf{B}\mathbf{y}_{k}$

 \bullet With $\|\boldsymbol{A}\| = \|\boldsymbol{W}^{1/2}\boldsymbol{A}\boldsymbol{W}^{1/2}\|_{\mathsf{F}}$ for a particular \boldsymbol{W}

$$\mathbf{B}^{(k+1)} = \left(\mathbb{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) \mathbf{B}^{(k)} \left(\mathbb{I} - \frac{\mathbf{s}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}\right) + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k^T \mathbf{s}_k}$$

- B^(k) ≻ 0 iff y^T_k s_k > 0 (Curvature Condition) ⇒ Guaranteed by appropriate line search, e.g., Armijo + (strong) Wolfe
- Under strong convexity (or if iterates satisfy certain properties), asymptotic super-linear rate of convergence

Quasi-Newton Method: Limited Memory

General QNM Update:

$\mathbf{B}^{(k+1)} = \mathbf{B}^{(k)} + [\text{something}]$

- **Problem:** Memory storage is $\mathcal{O}(d^2)$
- **Soution:** Limited-Memory QNMs, which are low-storage methods

L-BFGS

Instead of storing the inverse Hessian $\mathbf{B}^{(k)}$, L-BFGS maintains a history of iterates and gradients as

$$\{ \mathbf{s}_{k-m}, \mathbf{s}_{k-m-1}, \ldots, \mathbf{s}_{k} \},$$

 $\{ \mathbf{y}_{k-m}, \mathbf{y}_{k-m-1}, \ldots, \mathbf{y}_{k} \}.$

• $\mathbf{B}^{(k)}$ depends on $\mathbf{B}^{(k-1)}$, \mathbf{y}_{k-1} and \mathbf{s}_{k-1} .

•
$$\mathbf{B}^{(k-1)}$$
 depends on $\mathbf{B}^{(k-2)}$, \mathbf{y}_{k-2} and \mathbf{s}_{k-2} .

- and so on...
- So define $\mathbf{B}^{(k-1)}$ implicitly in terms of $\mathbf{B}^{(k-1)}$, \mathbf{y}_{k-2} and \mathbf{s}_{k-2} .
- We continue up to $\mathbf{B}^{(k-m)}$, which is initialized to be $\gamma \mathbb{I}$.
- These are used to implicitly do $\mathbf{B}^{(k)}$ -vector products.
- Linear rate of convergence

L-BFGS

Curvature Condition: $\left\langle \nabla f(\mathbf{x}^{(k+1)}) - \nabla f(\mathbf{x}^{(k)}), \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} \right\rangle > 0$

- If $f(\mathbf{x})$ is (strictly) convex \Longrightarrow
- Otherwise, (strong) Wolfe-condition on α (nonlinear inequality)

$$\langle
abla f(\mathbf{x} + lpha \mathbf{p}), \mathbf{p}
angle \geq eta \langle
abla f(\mathbf{x}), \mathbf{p}
angle, \ eta < 1$$

• When $\mathbf{g} \approx \nabla f \Longrightarrow$ noisy curvature estimate \Longrightarrow many issues arise!

L-BFGS [Byrd et al., 2014]

 Decoupling of the stochastic gradient and curvature estimations => different sample subsets for estimating y_k

•
$$\mathbf{s}_k = \bar{\mathbf{x}}_k - \bar{\mathbf{x}}_{k-1}$$
 where $\bar{\mathbf{x}}_k = \frac{1}{L} \sum_{j=k-L+1}^k \mathbf{x}^{(j)}$.

•
$$\mathbf{y}_k = \nabla^2 f_{\mathcal{S}_{\mathbf{H}}}(\bar{\mathbf{x}}_k) \mathbf{s}_k \approx \nabla f_{\mathcal{S}_{\mathbf{H}}}(\bar{\mathbf{x}}_k) - \nabla f_{\mathcal{S}_{\mathbf{H}}}(\bar{\mathbf{x}}_{k-1}).$$

- Update $\mathbf{H}^{(k)}$ every $L \ge 1$ iterations
- Under strong convexity, they show that $0 \prec \mu_1 \mathbf{I} \preceq \mathbf{H}^{(k)} \preceq \mu_2 \mathbf{I}$
- Setting $\alpha_k \propto 1/k$, they show

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^{\star})) \leq C/k$$

L-BFGS [Mokhtari and Ribeiro, 2014]

•
$$\mathbf{s}_k = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}$$

- Enforce gradient consistency, i.e., use the samples S: $\mathbf{y}_k = \nabla f_S(\mathbf{x}^{(k+1)}) - \nabla f_S(\mathbf{x}^{(k)}).$
- For some $\delta > 0$, $\widehat{\mathbf{y}}_k = \mathbf{y}_k \delta \mathbf{s}_k$
- Update \mathbf{B}_{k+1} as in the usual case with \mathbf{s}_k and $\hat{\mathbf{y}}_k$
- Add regularization: $\widehat{\mathbf{B}}_{k+1} = \mathbf{B}_{k+1} + m\mathbf{I}$
- Add regularization again: $\left(\widehat{\widehat{\mathbf{B}}}_{k+1}\right)^{-1} = \left(\widehat{\mathbf{B}}_{k+1}\right)^{-1} + M\mathbf{I}$
 - Spectrum of $\widehat{\widehat{\mathbf{B}}}_{k+1}$ is bounded above and away from zero
- Strong convexity of each f_i
- $\delta < \min_{\mathbf{x}} \lambda_{\min}(\nabla^2 f_i(\mathbf{x})) \Longrightarrow$ curvature condition holds
- Setting $lpha_k \propto 1/k$, they show

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^{\star})) \leq C/k$$

L-BFGS [Moritz et al., 2015]

- Combine the ideas of [Byrd et al., 2014] with variance reduction of [Johnson and Zhang, 2013]
 - **Recall SVRG**: For *s* and *k*, inner and outer iteration counters, respectively, estimate the gradient as

$$\mathbf{g}^{(s)} = \left(\nabla f_j(\mathbf{x}^{(s)}) - \nabla f_j(\mathbf{x}^{(k)}) + \nabla F(\mathbf{x}^{(k)})\right)$$

- No need to diminish step-size any more!
- Under strong convexity:

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^{\star})) \leq
ho^k \mathbb{E}(f(\mathbf{x}^{(0)}) - f(\mathbf{x}^{\star})), \quad
ho < 1$$

• As in SVRG, convergence is with respect to the outer iterations

L-BFGS [Berahas et al., 2016, Berahas and Takáč, 2017]

- Idea: Perform QN update on overlapping consecutive batches
- Idea: $\mathcal{T}_k = \mathcal{S}_k \cap \mathcal{S}_{k+1} \neq \emptyset$
- $\mathbf{y}_k = \nabla f_{\mathcal{O}_k}(\mathbf{x}^{(k+1)}) \nabla f_{\mathcal{O}_k}(\mathbf{x}^{(k)})$
- Using constant step-size α
 - Strongly convex:

$$\mathbb{E}(f(\mathbf{x}^{(k)}) - f(\mathbf{x}^{\star})) \le \rho^{k} \left(f(\mathbf{x}^{(0)}) - f(\mathbf{x}^{\star})\right) + \mathcal{O}(\alpha)$$

• Non-convex: Skip updating $\mathbf{H}^{(k)}$ if $\mathbf{y}_k^T \mathbf{s}_k \le \epsilon \|\mathbf{s}_k\|^2$

$$\mathbb{E}\left(\frac{1}{T}\sum_{k=0}^{T-1}\left\|\nabla f(\mathbf{x}^{(k)})\right\|^{2}\right) \leq \mathcal{O}\left(\frac{1}{T\alpha}\right) + \mathcal{O}(\alpha)$$

If $\alpha \leq \mathcal{O}(1/\sqrt{T}) \Longrightarrow \min_{k \leq T-1} \mathbb{E}\left\|\nabla f(\mathbf{x}^{(k)})\right\|^{2} \leq \mathcal{O}\sqrt{\frac{1}{T}}$

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Problem

$$\min_{\mathbf{x}\in\mathcal{R}^d}F(\mathbf{x})=\boldsymbol{f}(\mathbf{h}(\mathbf{x}))$$

•
$$\mathbf{h}: \mathcal{R}^d \to \mathcal{R}^p$$

• $f : \mathcal{R}^p \to \mathcal{R}$, and <u>convex</u>

Let
$$\mathsf{J}_\mathsf{h}:\mathcal{R}^d o\mathcal{R}^p$$
 be the Jacobian of h , i.e., $\mathsf{J}_\mathsf{h}(\mathsf{x})\in\mathcal{R}^{p imes d}$

$$\nabla F(\mathbf{x}) = \mathbf{J}_{\mathbf{h}}^{\mathsf{T}}(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))$$

$$\nabla^{2} F(\mathbf{x}) = \mathbf{J}_{\mathbf{h}}^{\mathsf{T}}(\mathbf{x}) \nabla^{2} f(\mathbf{h}(\mathbf{x})) \mathbf{J}_{\mathbf{h}}(\mathbf{x}) + \partial^{2} \mathbf{h}(\mathbf{x}) \nabla f(\mathbf{h}(\mathbf{x}))$$

(Generalized) Gauss-Newton Matrix:

$$\nabla^2 F(\mathbf{x}) \approx \underbrace{\mathbf{J}_{\mathbf{h}}^{\mathsf{T}}(\mathbf{x}) \nabla^2 f(\mathbf{h}(\mathbf{x})) \mathbf{J}_{\mathbf{h}}(\mathbf{x})}_{\mathbf{G}(\mathbf{x}) \triangleq \text{Gauss-Newton Matrix}} \succeq 0$$

(Generalized) Gauss-Newton Update:

$$\mathbf{G}(\mathbf{x}^{(k)})\mathbf{p} \approx -\nabla F(\mathbf{x}^{(k)})$$

Another interpretation:

$$f(\mathbf{h}(\mathbf{x})) \approx f\left(\mathbf{h}(\mathbf{x}^{(k)}) + \mathbf{J}_{\mathbf{h}}(\mathbf{x}^{(k)})\left(\mathbf{x} - \mathbf{x}^{(k)}\right)\right) \triangleq \boldsymbol{\ell}(\mathbf{x}; \mathbf{x}^{(k)})$$

$$\nabla f(\mathbf{h}(\mathbf{x}^{(k)})) = \nabla \boldsymbol{\ell}(\mathbf{x}^{(k)}; \mathbf{x}^{(k)}) = \mathbf{J}_{\mathbf{h}}^{\mathsf{T}}(\mathbf{x}^{(k)}) \nabla f(\mathbf{h}(\mathbf{x}^{(k)}))$$

 $\nabla^2 f(\mathbf{h}(\mathbf{x}^{(k)})) \approx \nabla^2 \boldsymbol{\ell}(\mathbf{x}^{(k)}; \mathbf{x}^{(k)}) = \mathbf{J}_{\mathbf{h}}^{\mathsf{T}}(\mathbf{x}^{(k)}) \nabla^2 f(\mathbf{h}(\mathbf{x}^{(k)})) \mathbf{J}_{\mathbf{h}}(\mathbf{x}^{(k)}) = \mathbf{G}(\mathbf{x}^{(k)})$

(Generalized) Gauss-Newton Matrix

$$abla^2 F(\mathbf{x}) \approx \mathbf{J}_{\mathbf{h}}^T(\mathbf{x}) \nabla^2 f(\mathbf{h}(\mathbf{x})) \mathbf{J}_{\mathbf{h}}(\mathbf{x})$$

Properties:

- **G**(**x**) ≽ 0, ∀**x**
- In some applications, after computing
 ∇F(x) = J^T_h(x)∇f(h(x)), the approximation G(x) does not
 involve any additional derivative evaluations
- G(x) is a good approximation if ||∂²h(x)∇f(h(x))|| is small, i.e.,
 - $\|\nabla f(\mathbf{h}(\mathbf{x}))\|$ is small, or
 - $\|\partial^2 \mathbf{h}(\mathbf{x})\|$ is small, i.e., **h** is nearly affine

Gauss-Newton Convergence

Under some regularity assumptions:

- Damped Gauss-Newton is globally convergent, i.e., $\lim_{k\to\infty} \left\| \nabla F(\mathbf{x}^{(k)}) \right\| = 0$
- The rate of convergence can be shown to be linear
- Local convergence $(\mathbf{S}(\mathbf{x}) \triangleq \partial^2 \mathbf{h}(\mathbf{x}^*) \nabla f(\mathbf{h}(\mathbf{x}^*)))$:

$$\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^{\star}\right\| \leq \left\|\mathbf{G}(\mathbf{x}^{\star})\right\| \left\|\mathbf{S}(\mathbf{x}^{\star})\right\| \left\|\mathbf{x}^{(k)} - \mathbf{x}^{\star}\right\| + \mathcal{O}\left(\left\|\mathbf{x}^{(k)} - \mathbf{x}^{\star}\right\|^{2}\right),$$

Finite-Sum Problem

$$\min_{\mathbf{x}\in\mathcal{R}^d}F(\mathbf{x})=\sum_{i=1}^n f_i(\mathbf{h}_i(\mathbf{x}))$$

- Machine Learning (e.g., deep/recurrent/reinforcement learning): [Martens, 2010, Martens and Sutskever, 2011, Chapelle and Erhan, 2011, Wu et al., 2017, Botev et al., 2017]... more on this later
- Scientific Computing (e.g., PDE inverse-problems): [Doel and Ascher, 2012, Roosta et al., 2014b, Roosta et al., 2014a, Roosta et al., 2015, Haber et al., 2000, Haber et al., 2012]
PDE Inverse Problems with Many R.H.S

$$\begin{array}{l} \nabla \cdot (\mathbf{x}(\mathbf{z}) \nabla u_i(\mathbf{z})) = q_i(\mathbf{z}), \quad \mathbf{z} \in \Omega \\ \\ \frac{\partial u_i(\mathbf{z})}{\partial \nu} = 0, \qquad \qquad \mathbf{z} \in \partial \Omega \end{array} \right\}, i = 1, \dots, n, \ \Omega \subset \mathcal{R}^2 \ \text{or} \ \mathcal{R}^3 \end{array}$$



(a) True x: 2D

(b) True x: 3D

Forward Problem

Discretize-Then-Optimize

$$\mathbf{v}_i = P_i A^{-1}(\mathbf{x}) \mathbf{q}_i + \boldsymbol{\epsilon}_i, \quad i = 1, 2, \dots, \mathbf{x} \in \mathcal{R}^d$$

- n: No. of measurements
- d: Mesh size

Intro Line-Search Based Methods Trust-Region Based Methods Discussion and Examples

Inverse Problem

Calculating " $\mathbf{A}^{-1}(\mathbf{x})\mathbf{q}_i$ " for each *i* is costly!

Intro Line-Search Based Methods Trust-Region Based Methods Discussion and Examples

A remedy: SAA

$$\begin{split} \mathcal{S} &\subset [n] \& |\mathcal{S}| = s \\ & \Downarrow \\ \mathcal{F}(\mathbf{x}) \approx \hat{\mathcal{F}}_{s}(\mathbf{x}) = \frac{1}{|\mathcal{S}|} \sum_{i \in \mathcal{S}} \|\mathbf{\Sigma}_{i}^{-\frac{1}{2}} \left(\mathbf{P}_{i} \mathbf{A}^{-1}(\mathbf{x}) \mathbf{q}_{i} - \mathbf{v}_{i}\right)\|_{2}^{2} \end{split}$$

Trace estimation: [Roosta and Ascher, 2015, Roosta et al., 2015]

Find *s* such that, for a given ϵ and δ , we get

$$\mathsf{Pr}\left(|\hat{\mathcal{F}}_{\boldsymbol{s}}(\mathbf{x}) - \mathcal{F}(\mathbf{x})| \leq \epsilon \mathcal{F}(\mathbf{x})
ight) \geq 1 - \delta$$

n = $\overline{961}$, Noise 1%, $\sigma_1 = 0.1$, $\sigma_2 = 1$

Method	Vanilla	Sub-Sampled
PDE Solves	128,774	3,921





(c) True Model

(d) Sub-Sampled GN

n = 512, Noise 2% $\sigma_I = 1$, $\sigma_{II} = .1$

Method	Vanilla	Sub-Sampled
PDE Solves	45,056	2,264



(e) True Model

(f) Sub-Sampled GN

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Cross Entropy Minimization

For $p_x(z)$, a density parametrized by x, the **cross-entropy minimization** with respect to a target density, $p_x(z)$, is

$$\min_{\mathbf{x}\in\mathcal{X}}\mathcal{L}(\mathbf{x}) = -\mathbb{E}_{\mathbf{x}}(\log p_{\mathbf{x}}(\mathbf{z})) = -\int p_{\mathbf{x}}(\mathbf{z})\log p_{\mathbf{x}}(\mathbf{z}) \,\mathrm{d}\mu(\mathbf{z}).$$

NB: $p_{\mathbf{x}}(\mathbf{z}) \mathrm{d} \boldsymbol{\mu}(\mathbf{z})$ can be the empirical measure over the training data.

Fisher Information Matrix

Suppose $\mathbb{Z} \sim p_x$. Under some weak regularity assumptions:

$$\mathbf{F}(\mathsf{x}) \triangleq \mathbb{E}_{\mathsf{x}}\left(\nabla \log p_{\mathsf{x}}(\mathbf{z}) \left(\nabla \log p_{\mathsf{x}}(\mathbf{z})\right)^{\mathcal{T}}\right) = -\mathbb{E}_{\mathsf{x}}\left(\nabla^2 \log p_{\mathsf{x}}(\mathbf{z})\right).$$

Natural Gradient Descent

$$\mathbf{F}(\mathbf{x}^{(k)})\mathbf{p}^{(k)} \approx \mathbf{g}^{(k)} \Longrightarrow \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)}\mathbf{p}^{(k)}$$

Interpretation I:

$$\min_{\mathbf{x}\in\mathcal{X}}\mathcal{L}(\mathbf{x}) = -\mathbb{E}_{\mathbf{x}}\left(\log p_{\mathbf{x}}(\mathbf{z})\right)$$

Natural Gradient vs. Newton's Method

For a given **x**:

$$\begin{array}{lll} \text{Hessian Matrix:} \quad \nabla^{2}\mathcal{L}(\mathbf{x}) &= -\mathbb{E}_{\mathbf{x}}\left(\nabla^{2}\log p_{\mathbf{x}}(\mathbf{z})\right)\\ \text{Fisher Matrix:} \quad \mathbf{F}(\mathbf{x}) &= -\mathbb{E}_{\mathbf{x}}\left(\nabla^{2}\log p_{\mathbf{x}}(\mathbf{z})\right) \end{array}$$

Interpretation I:

Let $p_{\mathbf{x}}$ be the empirical measure over the given training set $\{\mathbf{z}_i\}_{i=1}^n$ where $\mathbf{z}_i \sim p_{\mathbf{x}^*}$ for some true, but unknown, parameter \mathbf{x}^* , i.e., empirical risk minimization:

$$\min_{\mathbf{x}\in\mathcal{X}}\mathcal{L}(\mathbf{x}) = -\frac{1}{n}\sum_{i=1}^{n}\log p_{\mathbf{x}}(\mathbf{z}_{i})$$

Approximation I: Natural Gradient vs. Newton's Method

For a given **x**:

Hessian:
$$\nabla^2 \mathcal{L}(\mathbf{x}) = -\frac{1}{n} \sum_{i=1}^n \nabla^2 \log p_{\mathbf{x}}(\mathbf{z}_i), \quad \mathbf{z}_i \sim p_{\mathbf{x}^*}$$

Approximate Fisher: $\hat{\mathbf{F}}(\mathbf{x}) = -\frac{1}{n} \sum_{i=1}^n \nabla^2 \log p_{\mathbf{x}}(\mathbf{z}_i), \quad \mathbf{z}_i \sim p_{\mathbf{x}}$

Interpretation II:

$$\min_{\mathsf{x}\in\mathcal{X}}\mathcal{L}(\mathsf{x}) = -\frac{1}{n}\sum_{i=1}^{n}\log p_{\mathsf{x}}(\mathsf{z}_{i})$$

In Gauss-Newton, we had $\mathcal{L}(\mathbf{x}) = f(h(\mathbf{x}))$. Here, we can consider $f(t) = -\log t \in \mathcal{R}$ and $h(\mathbf{x}) = p_{\mathbf{x}}(z) \in \mathcal{R}$. So, $\mathbf{G}(\mathbf{x}) = f''(h(\mathbf{x}))\nabla h(\mathbf{x})\nabla h(\mathbf{x})^T = \frac{1}{(p_{\mathbf{x}}(z))^2}\nabla p_{\mathbf{x}}(z) (\nabla p_{\mathbf{x}}(z))^T$ $= \left(\frac{1}{p_{\mathbf{x}}(z)}\nabla p_{\mathbf{x}}(z)\right) \left(\frac{1}{p_{\mathbf{x}}(z)}\nabla p_{\mathbf{x}}(z)\right)^T = \nabla \log p_{\mathbf{x}}(z) (\nabla \log p_{\mathbf{x}}(z))^T$

Approximation II: Natural Gradient vs. Gauss-Newton

$$\begin{split} \mathbf{G}(\mathbf{x}) &= -\frac{1}{n} \sum_{i=1}^{n} \nabla \log p_{\mathbf{x}}(\mathbf{z}_{i}) \left(\nabla \log p_{\mathbf{x}}(\mathbf{z}_{i}) \right)^{T}, \quad \mathbf{z}_{i} \sim p_{\mathbf{x}^{\star}} \\ \hat{\mathbf{F}}(\mathbf{x}) &= -\frac{1}{n} \sum_{i=1}^{n} \nabla \log p_{\mathbf{x}}(\mathbf{z}_{i}) \left(\nabla \log p_{\mathbf{x}}(\mathbf{z}_{i}) \right)^{T}, \quad \mathbf{z}_{i} \sim p_{\mathbf{x}} \end{split}$$

Interpretation III:

More generally, consider fitting probabilistic models

$$\min_{\mathbf{x}\in\mathcal{R}^d}\mathcal{L}(\mathbf{x})=L(p_{\mathbf{x}})$$

Recall: steepest descent in Euclidean space

Ideally, we want

$$\mathbf{p}^{\star} = \operatorname*{argmin}_{\|\mathbf{p}\| \leq 1} \mathcal{L}(\mathbf{x} + \mathbf{p}),$$

but it is easier to do

$$\frac{-\nabla \mathcal{L}(\mathbf{x})}{\|\nabla \mathcal{L}(\mathbf{x})\|} = \operatorname*{argmin}_{\|\mathbf{p}\| \leq 1} \langle \nabla \mathcal{L}(\mathbf{x}), \mathbf{p} \rangle$$

Interpretation III:

KullbackLeibler distance

For given **x** and **x**, the Kullback-Leibler distance from p_x to p_x is

$$\mathsf{KL}(\mathbf{x} \parallel \mathbf{x}) \triangleq \mathbb{E}_{\mathbf{x}}\left(\log \frac{p_{\mathbf{x}}(\mathbf{z})}{p_{\mathbf{x}}(\mathbf{z})}\right) = \int \left(\log \frac{p_{\mathbf{x}}(\mathbf{z})}{p_{\mathbf{x}}(\mathbf{z})}\right) p_{\mathbf{x}}(\mathbf{z}) \, \mathrm{d}\mu(\mathbf{z}).$$

$$\mathbf{F}(\mathbf{x}) = \nabla_{\mathbf{x}}^2 \, \mathbf{KL}(\mathbf{x} \parallel \mathbf{x})|_{\mathbf{x}=\mathbf{x}}$$

If $F(x) \succ 0$, then in a neighborhood of x, we have $KL(x \parallel x) > 0$, and

$$\mathsf{KL}(\mathbf{x} \parallel \mathbf{x}) \approx \frac{1}{2} (\mathbf{x} - \mathbf{x})^2 \, \mathsf{F}(\mathbf{x}) (\mathbf{x} - \mathbf{x})$$

Interpretation III:

Ideally, we want

$$\mathbf{p}^{\star} = \underset{\mathsf{KL}(\mathbf{x} \parallel \mathbf{x} + \mathbf{p}) \leq 1}{\operatorname{argmin}} \mathcal{L}(\mathbf{x} + \mathbf{p})$$

But, if $\boldsymbol{p}\ll 1,$ we can approximate

$$\mathbf{F}^{-1}(\mathbf{x})\nabla\mathcal{L}(\mathbf{x}) \propto \operatorname*{argmin}_{\mathbf{p}^{\mathcal{T}}\mathbf{F}(\mathbf{x})\mathbf{p}\leq 1} \langle \nabla\mathcal{L}(\mathbf{x}), \mathbf{p} \rangle$$

- Classical: [Amari, 1998]
- Overview: [Martens, 2014]
- On manifolds: [Song and Ermon, 2018]
- Deep learning: [Pascanu and Bengio, 2013, Martens and Grosse, 2015, Grosse and Salakhudinov, 2015]

Outline

- Part I: Convex
 - Smooth
 - Newton-CG
 - Non-Smooth
 - Proximal Newton
 - Semi-smooth Newton

• Part II: Non-Convex

- Line-Search Based Methods
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- Trust-Region Based Methods
 - Trust-Region
 - Cubic Regularization
- Part III: Discussion and Examples

Problem Statement

Minimizing Finite Sum Problem

$$\min_{\mathbf{x}\in\mathcal{X}\subseteq\mathbb{R}^d}F(\mathbf{x})=\frac{1}{n}\sum_{i=1}^nf_i(\mathbf{x})$$

- f_i : (non-)convex and smooth
- $n \gg 1$ and/or $d \gg 1$

• Trust Region: [Sorensen, 1982, Conn et al., 2000]

$$\mathbf{s}^{(k)} = \arg\min_{\|\mathbf{s}\| \le \Delta_k} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle$$

• Cubic Regularization: [Griewank, 1981, Nesterov et al., 2006, Cartis et al., 2011a, Cartis et al., 2011b]

$$\mathbf{s}^{(k)} = \arg\min_{\mathbf{s} \in \mathbb{R}^d} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle + \frac{\sigma_k}{3} \|\mathbf{s}\|^3$$

• Trust Region:

$$\mathbf{s}^{(k)} = \arg\min_{\|\mathbf{s}\| \le \Delta_k} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle$$

• Cubic Regularization:

$$\mathbf{s}^{(k)} = \arg\min_{\mathbf{s} \in \mathbb{R}^d} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \nabla^2 F(\mathbf{x}^{(k)}) \mathbf{s} \right\rangle + \frac{\sigma_k}{3} \|\mathbf{s}\|^3$$

• Trust Region:

$$\mathbf{s}^{(k)} = \arg\min_{\|\mathbf{s}\| \le \Delta_k} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \mathbf{H}^{(k)} \mathbf{s} \right\rangle$$

• Cubic Regularization:

$$\mathbf{s}^{(k)} = \arg\min_{\mathbf{s} \in \mathbb{R}^d} \left\langle \mathbf{s}, \nabla F(\mathbf{x}^{(k)}) \right\rangle + \frac{1}{2} \left\langle \mathbf{s}, \mathbf{H}^{(k)} \mathbf{s} \right\rangle + \frac{\sigma_k}{3} \|\mathbf{s}\|^3$$

• To get iteration complexity, previous work required:

$$\left\| \left(\mathbf{H}^{(k)} - \nabla^2 F(\mathbf{x}^{(k)}) \right) \mathbf{s}^{(k)} \right\| \le C \|\mathbf{s}^{(k)}\|^2 \tag{1}$$

• Stronger than "Dennis-Moré"

$$\lim_{k \to \infty} \frac{\| \left(H(\mathbf{x}(k)) - \nabla^2 F(\mathbf{x}(k)) \right) \mathbf{s}(k) \|}{\| \mathbf{s}(k) \|} = 0$$

• We relaxed (1) to

$$\left\| \left(\mathbf{H}^{(k)} - \nabla^2 F(\mathbf{x}^{(k)}) \right) \mathbf{s}^{(k)} \right\| \le \epsilon \|\mathbf{s}^{(k)}\|$$
(2)

• Quasi-Newton, Sketching, Sub-Sampling satisfy Dennis-Moré and (2) but not necessarily (1)

$$ig\| H(\mathbf{x}) -
abla^2 F(\mathbf{x}) ig\| \le \epsilon \implies ig\| (H(\mathbf{x}) -
abla^2 F(\mathbf{x})) \, \mathbf{s} ig\| \le \epsilon \|\mathbf{s}\|$$
 $H(\mathbf{x}) = rac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}}
abla^2 f_j(\mathbf{x})$

Lemma (Uniform Sampling [Xu et al., 2017])

Suppose
$$\|\nabla^2 f_i(\mathbf{x})\| \leq K_i$$
, $i = 1, 2, ..., n$. Let $\mathbf{K} = \max_{i=1,...,n} K_i$.
Given any $0 < \epsilon < 1$, $0 < \delta < 1$, and $\mathbf{x} \in \mathbb{R}^d$, if

$$|\mathcal{S}| \geq rac{16 \mathcal{K}^2}{\epsilon^2} \log rac{2d}{\delta},$$

then for

$$H(\mathbf{x}) = rac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}}
abla^2 f_j(\mathbf{x}),$$

we have

$$\Pr\left(\|H(\mathbf{x}) - \nabla^2 F(\mathbf{x})\| \le \epsilon\right) \ge 1 - \delta.$$

• Only top eigenvalues/eigenvectors need to preserved.

$$F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{a}_i^T \mathbf{x})$$

$$\mathbf{p}_i = \frac{|f_i''(\mathbf{a}_i^T \mathbf{x})| \|\mathbf{a}_i\|_2^2}{\sum_{j=1}^n |f_j''(\mathbf{a}_j^T \mathbf{x})| \|\mathbf{a}_j\|_2^2}$$

$$H(\mathbf{x}) = \frac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}} \frac{1}{n p_j} \nabla^2 f_j(\mathbf{x})$$

Lemma (Non-Uniform Sampling [Xu et al., 2017])

Suppose $\|\nabla^2 f_i(\mathbf{x})\| \leq K_i$, i = 1, 2, ..., n. Let $\overline{K} = \frac{1}{n} \sum_{i=1}^n K_i$. Given any $0 < \epsilon < 1$, $0 < \delta < 1$, and $\mathbf{x} \in \mathbb{R}^d$, if

$$|\mathcal{S}| \geq rac{16\overline{K}^2}{\epsilon^2}\lograc{2d}{\delta},$$

$$H(\mathbf{x}) = rac{1}{|\mathcal{S}|} \sum_{j \in \mathcal{S}} rac{1}{n p_j} \nabla^2 f_j(\mathbf{x}),$$

we have

$$\Pr\left(\|H(\mathbf{x}) - \nabla^2 F(\mathbf{x})\| \le \epsilon\right) \ge 1 - \delta,$$

 $\frac{1}{n}\sum_{i=1}^{n}K_{i}\leq \max_{i=1,\ldots,n}K_{i}$

Theorem ([Xu et al., 2017])

If $\epsilon \in \mathcal{O}(\epsilon_{H})$, then Stochastic TR terminates after

$$T \in \mathcal{O}\left(\max\{\epsilon_g^{-2}\epsilon_H^{-1}, \epsilon_H^{-3}\}\right),\,$$

iterations, upon which, with high probability, we have that

$$\|\nabla F(\mathbf{x})\| \leq \epsilon_g$$
, and $\lambda_{\min}(\nabla^2 F(\mathbf{x})) \geq -(\epsilon + \epsilon_H)$.

• This is tight! [Cartis et al., 2012]

Theorem ([Xu et al., 2017])

If $\epsilon \in \mathcal{O}(\epsilon_g, \epsilon_H)$, then Stochastic ARC terminates after

$$T \in \mathcal{O}\left(\max\{\epsilon_g^{-3/2}, \epsilon_H^{-3}\}
ight),$$

iterations, upon which, with high probability, we have that

$$\|
abla F(\mathbf{x})\| \leq \epsilon_g, \quad \textit{and} \quad \lambda_{\min}(
abla^2 F(\mathbf{x})) \geq -\left(\epsilon + \epsilon_H
ight).$$

• This is tight! [Cartis et al., 2012]

• For
$$\epsilon_H^2 = \epsilon_g = \epsilon$$

- Stochastic TR: $T \in \mathcal{O}(\epsilon^{-2.5})$
- Stochastic ARC: $T \in \mathcal{O}(\epsilon^{-1.5})$

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• Part III: Discussion and Examples

Intro Line-Search Based Methods Trust-Region Based Methods Discussion and Examples

But why 1st Order Methods?

- Q: But Why 1st Order Methods?
 - Cheap Iterations

• Easy To Implement

• "Good" Worst-Case Complexities

Good Generalization

But why Not?2nd Order Methods

- Q: But Why Not 2nd Order Methods?
 - Cheap Expensive Iterations
 - Æ≱≸y Hard To Implement
 - //G/d/// "Bad" Worst-Case Complexities
 - Øøø Bad Generalization

Our Goal...

- Goal: Improve 2nd Order Methods...
 - Cheap / k/p/e//s///e Iterations
 - Easy /////d To Use
 - "Good" //₿/#// Average(?)-Case Complexities
 - Good ₿ǿ Generalization

Our Goal ..

Any Other Advantages?

• Effective Iterations \Rightarrow Less Iterations \Rightarrow Less Communications

• Saddle Points For Non-Convex Problems

- Less Sensitive to Parameter Tuning
- Less Sensitive to Initialization

Intro Line-Search Based Methods Trust-Region Based Methods Discussion and Examples

Simulations: ℓ_2 Regularized LR

$$F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \left(\log \left(1 + \exp(\mathbf{a}_{i}^{T} \mathbf{x}) \right) - b_{i} \mathbf{a}_{i}^{T} \mathbf{x} \right) + \frac{\lambda}{2} \|\mathbf{x}\|^{2}$$

Data	п	р	NNZ	$\kappa(F)$
D_1	10 ⁶	10 ⁴	0.02%	$pprox 10^4$
<i>D</i> ₂	$5 imes 10^4$	$5 imes 10^3$	Dense	$pprox 10^{6}$
<i>D</i> ₃	107	$2 imes 10^4$	0.006%	$pprox 10^{10}$

Line-Search Based Methods Trust-Region Based Methods Discussion and Examples

 $D_1, n = 10^6, p = 10^4, \text{sparsity} : 0.02\%, \kappa \approx 10^4$


D_2 , $n = 5 \times 10^4$, $p = 5 \times 10^3$, sparsity : Dense, $\kappa \approx 10^6$



 $D_3, n = 10^7, p = 2 \times 10^4, \text{sparsity} : 0.006\%, \kappa \approx 10^{10}$



Newton GPU vs. TensorFlow

Data: Cover Type, $n = 4.5 \times 10^5, d = 378$



Newton GPU vs. TensorFlow

Data: Newsgroup20, $n = 10^4$, $d = 10^6$















Numerical Examples: Deep Learning

Dataset	Size	Network	(# parameters)
curves	20,000	784-400-200-100-50-25-6	842, 340
Cifar10	50,000	ResNet18	270,896

Deep Auto-Encoder



Figure: Random Initialization

Deep Auto-Encoder



Figure: Random Initialization

Deep Auto-Encoder



Figure: Zero Initialization

Deep Auto-Encoder



Figure: Zero Initialization

Deep Auto-Encoder



Figure: Scaled Random Initialization

Deep Auto-Encoder



Figure: Scaled Random Initialization



Is it all rosie?

ResNet18



No Batch Normalization + No data augmentation.

ResNet18



Batch Normalization + Data augmentation.

Worst Case Complexity

My to pick with worst case complexity results!!!









- Q: What do "Newton's method" and "air travel" have in common?
- A: Both are very fast, but their worst-case is bad!!!



Should you ask a Question during Seminar?



THANK YOU!

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