

Krylov Cubic Regularized Newton: A Subspace Second-Order Method with Dimension-Free Convergence Rate

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Outline

- ① Introduction
- ② The Proposed Method
- ③ Convergence Analysis
- ④ Numerical Results

Convex Minimization

- Consider the unconstrained minimization problem

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where f is **convex** and **twice continuously differentiable**

- Popular methods: **first-order methods** such as gradient descent

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \eta \nabla f(\mathbf{x}_k)$$

- Cheap to implement ✓
- Slow convergence, esp. for ill-conditioned problems ✗

Second-Order Methods

- ▶ We focus on second-order methods that utilize the **Hessian of f**
- ▶ Newton's method

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- ▶ Cubic regularized Newton (CRN) method [[Griewank'81](#); [Nesterov-Polyak'06](#)]

$$\mathbf{x}_{k+1} = \operatorname{argmin}_{\mathbf{x} \in \mathbb{R}^d} \left\{ f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^\top (\mathbf{x} - \mathbf{x}_k) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_k)^\top \nabla^2 f(\mathbf{x}_k) (\mathbf{x} - \mathbf{x}_k) + \frac{M}{6} \|\mathbf{x} - \mathbf{x}_k\|^3 \right\}$$

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- When f is convex, $f(\mathbf{x}_k) - f^* = \mathcal{O}(1/k^2)$
- When f is strongly convex, it achieves a superlinear convergence rate

The Curse of Dimensionality

- ▶ The main drawback of CRN is its substantial memory and computational costs
 - Computing & storing the Hessian $\nabla^2 f(\mathbf{x})$: $\mathcal{O}(d^2)$
 - Solving a cubic subproblem: $\mathcal{O}(d^3)$
- ▶ As a result, CRN becomes impractical for optimization problems with high dimensions

Subspace Second-Order Methods

- To reduce the cost, one approach is to execute 2nd-order updates in a subspace $\mathcal{V}_k$ of dimension $m \ll d$ [Doikov-Richtárik'18; Gower et al.'19; Hanzely et al.'20]

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CRN:

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- ▶ Equivalently, let $\mathbf{V}_k \in \mathbb{R}^{d \times m}$ whose columns form an orthonormal basis for $\mathcal{V}_k$

Subspace CRN:

$$\mathbf{z}_k = \operatorname{argmin}_{\mathbf{z} \in \mathbb{R}^m} \left\{ \tilde{\mathbf{g}}_k^\top \mathbf{z} + \frac{1}{2} \mathbf{z}^\top \tilde{\mathbf{H}}_k \mathbf{z} + \frac{M}{6} \|\mathbf{z}\|^3 \right\}, \quad \mathbf{s}_k = \mathbf{V}_k \mathbf{z}_k,$$

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 - Randomized Block Cubic Newton (RBCN) [Doikov-Richtárik'18]:
Sampling a random block of m coordinates
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*Question: Can we improve the **dimensional dependence** of subspace second-order methods?*

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- ▶ Intuitively, it stems from the fact that the subspace is chosen **uniformly random**, oblivious to the objective function f
- ▶ Such a random subspace is unlikely to contain a **“good” descent direction**
- ▶ It should be better to employ a subspace customized to the **local geometry of f**

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Methods	Per-iteration cost	Convergence rate
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Krylov CRN (ours)	$\mathcal{O}(md)^{**}$	$\mathcal{O}(\frac{1}{mk} + \frac{1}{k^2})$

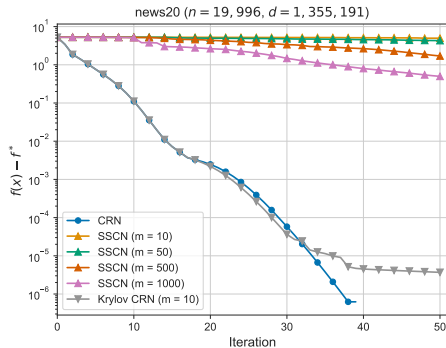
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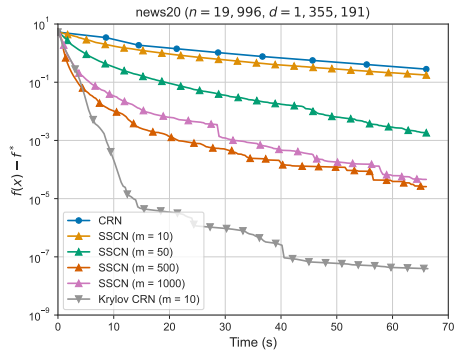
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- ▶ When the Hessian spectrum possesses certain structure, our method can achieve a faster rate

Contributions



(a) Loss curve by iteration



(b) Loss curve by time

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Review: Cubic Regularized Newton Method

► We assume that:

- $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is **convex**
- f is **bounded from below** and has **bounded level-sets**
- The Hessian of f is **Lipchitz**, i.e., $\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \leq L_2 \|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

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► An important property: upper bound on **quadratic approximation error**

$$\left| f(\mathbf{x}) - \left(f(\mathbf{x}_k) + \mathbf{g}_k^\top (\mathbf{x} - \mathbf{x}_k) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_k)^\top \mathbf{H}_k (\mathbf{x} - \mathbf{x}_k) \right) \right| \leq \frac{L_2}{6} \|\mathbf{x} - \mathbf{x}_k\|^3, \quad \forall \mathbf{x} \in \mathbb{R}^d$$

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► The CRN selects $\mathbf{x}_{k+1}$ as the minimizer of the **cubic upper approximation**

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Review: Cubic Regularized Newton Method

Theorem

Let $\{\mathbf{x}_k\}_{k \geq 0}$ be generated by CRN and define $D := \sup\{\|\mathbf{x} - \mathbf{x}^*\| : \mathbf{x} \in \mathbb{R}^d, f(\mathbf{x}) \leq f(\mathbf{x}_0)\}$. Then we have

$$f(\mathbf{x}_k) - f^* \leq \frac{9L_2 D^3}{(k+2)(k+1)}$$

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- Choosing $\mathbf{s} = \frac{3}{k+3}(\mathbf{x}^* - \mathbf{x}_k)$ and using **convexity of f** :

$$f(\mathbf{x}_{k+1}) \leq f\left(\frac{k}{k+3}\mathbf{x}_k + \frac{3}{k+3}\mathbf{x}^*\right) + \frac{9L_2\|\mathbf{x}_k - \mathbf{x}^*\|^3}{(k+3)^3} \leq \frac{k}{k+3}f(\mathbf{x}_k) + \frac{3}{k+3}f^* + \frac{9L_2D^3}{(k+3)^3}$$

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- ▶ Define $A_k = k(k+1)(k+2)$:

$$f(\mathbf{x}_{k+1}) - f^* \leq \frac{k}{k+3}(f(\mathbf{x}_k) - f^*) + \frac{9L_2D^3}{(k+3)^3}$$

$$\Rightarrow A_{k+1}(f(\mathbf{x}_{k+1}) - f^*) \leq A_k(f(\mathbf{x}_k) - f^*) + 9L_2D^3$$

$$\Rightarrow A_{k+1}(f(\mathbf{x}_{k+1}) - f^*) \leq 9L_2D^3(k+1) \quad \Rightarrow \quad f(\mathbf{x}_{k+1}) - f^* \leq \frac{9L_2D^3}{(k+2)(k+3)}$$

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$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \mathbf{g}_k^\top \mathbf{s} + \frac{1}{2} \mathbf{s}^\top \mathbf{H}_k \mathbf{s} + \frac{L_2}{6} \|\mathbf{s}\|^3, \quad \cancel{\forall \mathbf{s} \in \mathbb{R}^d} \quad \forall \mathbf{s} \in \mathcal{V}_k$$

Subspace Cubic Regularized Newton

- Subspace CRN:

$$\mathbf{s}_k = \operatorname{argmin}_{\mathbf{s} \in \mathcal{V}_k} \left\{ \mathbf{g}_k^\top \mathbf{s} + \frac{1}{2} \mathbf{s}^\top \mathbf{H}_k \mathbf{s} + \frac{L_2}{6} \|\mathbf{s}\|^3 \right\}$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$$

- Where the analysis would break when introducing the subspace $\mathcal{V}_k$?
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- Let $\mathbf{P}_k := \mathbf{V}_k \mathbf{V}_k^\top$ be the orthogonal projection matrix of $\mathcal{V}_k$. Since $\mathbf{P}_k \mathbf{s} \in \mathcal{V}_k$, $\forall \mathbf{s} \in \mathbb{R}^d$:

$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \mathbf{g}_k^\top \mathbf{P}_k \mathbf{s} + \frac{1}{2} (\mathbf{P}_k \mathbf{s})^\top \mathbf{H}_k (\mathbf{P}_k \mathbf{s}) + \frac{L_2}{6} \|\mathbf{P}_k \mathbf{s}\|^3, \quad \forall \mathbf{s} \in \mathbb{R}^d$$

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► The exactly same analysis would apply if, for any $\mathbf{s} \in \mathbb{R}^d$,

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- Combining (A) and (B), we obtain that

$$\mathbf{g}_k \in \mathcal{V}_k, \mathbf{H}_k \mathbf{g}_k \in \mathcal{V}_k, \mathbf{H}_k^2 \mathbf{g}_k \in \mathcal{V}_k, \dots, \Rightarrow \text{span}\{\mathbf{H}_k^i \mathbf{g}_k \mid i = 0, 1, \dots\} \subset \mathcal{V}_k$$

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(B) $(\mathbf{P}_k \mathbf{s})^\top \mathbf{H}_k (\mathbf{P}_k \mathbf{s}) \leq \mathbf{s}^\top \mathbf{H}_k \mathbf{s} \Leftrightarrow \mathbf{P}_k \mathbf{H}_k \mathbf{P}_k \preceq \mathbf{H}_k \Leftrightarrow \mathbf{H}_k \mathbf{v} \in \mathcal{V}_k, \forall \mathbf{v} \in \mathcal{V}_k$

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- This is exactly the maximal Krylov subspace generated by $\mathbf{H}_k$ and $\mathbf{g}_k$!

Krylov Subspace

- Formally, the j -th Krylov subspace generated by $\mathbf{A} \in \mathbb{R}^{d \times d}$ and $\mathbf{b} \in \mathbb{R}^d$ is defined as

$$\mathcal{K}_j(\mathbf{A}, \mathbf{b}) = \text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \dots, \mathbf{A}^{j-1}\mathbf{b}\}.$$

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- Moreover, there exists an integer $r_0 \leq d$ such that:

$$\mathcal{K}_1(\mathbf{A}, \mathbf{b}) \subset \mathcal{K}_2(\mathbf{A}, \mathbf{b}) \subset \dots \subset \underbrace{\mathcal{K}_{r_0}(\mathbf{A}, \mathbf{b})}_{\text{dim}=r_0} = \mathcal{K}_{r_0+1}(\mathbf{A}, \mathbf{b}) = \mathcal{K}_{r_0+2}(\mathbf{A}, \mathbf{b}) = \dots$$

We call $\mathcal{K}_{r_0}(\mathbf{A}, \mathbf{b})$ the maximal Krylov subspace

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- To sum up: if we let $\mathcal{V}_k = \mathcal{K}_{r_0}(\mathbf{H}_k, \mathbf{g}_k)$, the subspace CRN retains the same convergence rate of CRN

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- To sum up: if we let $\mathcal{V}_k = \mathcal{K}_{r_0}(\mathbf{H}_k, \mathbf{g}_k)$, the subspace CRN retains the same convergence rate of CRN
- However, r_0 can be as large as $d \Rightarrow$ we use the Krylov subspace up to dim m

► Let us check if $\mathcal{V}_k = \mathcal{K}_m(\mathbf{H}_k, \mathbf{g}_k)$ satisfies the three conditions:

(A) $\mathbf{g}_k^\top \mathbf{P}_k \mathbf{s} \leq \mathbf{g}_k^\top \mathbf{s} \iff \mathbf{g}_k \in \mathcal{V}_k$

(B) $(\mathbf{P}_k \mathbf{s})^\top \mathbf{H}_k (\mathbf{P}_k \mathbf{s}) \leq \mathbf{s}^\top \mathbf{H}_k \mathbf{s} \iff \mathbf{H}_k \mathbf{v} \in \mathcal{V}_k, \forall \mathbf{v} \in \mathcal{V}_k$

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Krylov Subspace

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- Only need to control the error from Condition (B)
- In comparison, when $\mathcal{V}_k$ is chosen randomly, both (A) and (B) only hold approximately and the induced errors depend on m/d

Krylov Cubic Regularized Newton

► **Input:** Initial point $\mathbf{x}_0 \in \mathbb{R}^d$, subspace dimension m , regularization parameter $M > 0$

► **for** $k = 0, 1, \dots$, **do**

- $\mathbf{V}_k \leftarrow$ the orthonormal basis of $\mathcal{K}_m(\mathbf{H}_k, \mathbf{g}_k)$, $\tilde{\mathbf{g}}_k \leftarrow \mathbf{V}_k^\top \mathbf{g}_k$, $\tilde{\mathbf{H}}_k \leftarrow \mathbf{V}_k^\top \mathbf{H}_k \mathbf{V}_k$
- Solve the cubic subproblem

$$\mathbf{z}_k = \operatorname{argmin}_{\mathbf{z} \in \mathbb{R}^m} \left\{ \tilde{\mathbf{g}}_k^\top \mathbf{z} + \frac{1}{2} \mathbf{z}^\top \tilde{\mathbf{H}}_k \mathbf{z} + \frac{M}{6} \|\mathbf{z}\|^3 \right\},$$

- Update $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{V}_k \mathbf{z}_k$

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► **end for**

► The remaining question: How to compute $\mathbf{V}_k$, $\tilde{\mathbf{g}}_k$, and $\tilde{\mathbf{H}}_k$?

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► **end for**

► The remaining question: How to compute $\mathbf{V}_k$, $\tilde{\mathbf{g}}_k$, and $\tilde{\mathbf{H}}_k$? $\Leftarrow$ Lanczos method!

Lanczos Method

- ▶ **Input:** $\mathbf{H} \in \mathbb{R}^{d \times d}$, $\mathbf{g} \in \mathbb{R}^d$, and the dimension m
- ▶ **Initialize:** $\mathbf{v}_1 = \mathbf{g}/\|\mathbf{g}\|$, $\beta_1 = 0$, $\mathbf{v}_0 = 0$
- ▶ **for** $j = 1, 2, \dots, m$ **do**
 - $\mathbf{w}_j \leftarrow \mathbf{H}\mathbf{v}_j - \beta_j\mathbf{v}_{j-1}$ // one Hessian-vector product (HVP)
 - $\alpha_j \leftarrow \mathbf{w}_j^\top \mathbf{v}_j$
 - $\mathbf{w}_j \leftarrow \mathbf{w}_j - \alpha_j\mathbf{v}_j$
 - $\beta_{j+1} \leftarrow \|\mathbf{w}_j\|_2$
 - $\mathbf{v}_{j+1} \leftarrow \mathbf{w}_j/\beta_{j+1}$
- ▶ **end for**
- ▶ **Output:** $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m]$, $\tilde{\mathbf{g}} = \|\mathbf{g}\|\mathbf{e}_1$, and $\tilde{\mathbf{H}} =$

$$\begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \ddots & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ & & & & \beta_m & \alpha_m \end{bmatrix}$$

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- ▶ No need to compute & store $\mathbf{H}$ explicitly; only requires m HVPs
 $\Rightarrow$ Can be done efficiently via back-propagation [Pearlmutter'94]

Lanczos Method

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- ▶ **for** $j = 1, 2, \dots, m$ **do**
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- ▶ **end for**
- ▶ **Output:** $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m]$, $\tilde{\mathbf{g}} = \|\mathbf{g}\| \mathbf{e}_1$, and $\tilde{\mathbf{H}} =$

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- ▶ No need to compute & store $\mathbf{H}$ explicitly; only requires m HVPs
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- ▶ Bonus: $\tilde{\mathbf{H}}$ is a sparse tridiagonal matrix

Krylov Cubic Regularized Newton

- ▶ **Input:** Initial point $\mathbf{x}_0 \in \mathbb{R}^d$, subspace dimension m , regularization parameter $M > 0$
- ▶ **for** $k = 0, 1, \dots$, **do**

- $(\mathbf{V}_k, \tilde{\mathbf{g}}_k, \tilde{\mathbf{H}}_k) \leftarrow \text{LANCZOS}(\mathbf{H}_k, \mathbf{g}_k; m)$
- Solve the cubic subproblem

$$\mathbf{z}_k = \operatorname{argmin}_{\mathbf{z} \in \mathbb{R}^m} \left\{ \tilde{\mathbf{g}}_k^\top \mathbf{z} + \frac{1}{2} \mathbf{z}^\top \tilde{\mathbf{H}}_k \mathbf{z} + \frac{M}{6} \|\mathbf{z}\|^3 \right\},$$

- Update $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{V}_k \mathbf{z}_k$

- ▶ **end for**

- ▶ Per-iteration computational cost

- Performing Lanczos iteration: m HVPs $\Rightarrow \mathcal{O}(md)$
- Solving the cubic subproblem: $\mathcal{O}(m)$

Outline

- ① Introduction
- ② The Proposed Method
- ③ Convergence Analysis
- ④ Numerical Results

Convergence Analysis

- For simplicity, we further assume that $\nabla^2 f(\mathbf{x}) \preceq L_1 \mathbf{I}$ as in [\[Hanzely et al.'20\]](#)

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- For simplicity, we further assume that $\nabla^2 f(\mathbf{x}) \preceq L_1 \mathbf{I}$ as in [Hanzely et al.'20]

Lemma

Let $\{\mathbf{x}_k\}$ be generated by Krylov CRN with subspace dim m . We have

$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \mathbf{g}_k^\top \mathbf{s} + \frac{1}{2} \mathbf{s}^\top \mathbf{H}_k \mathbf{s} + \frac{L_2}{6} \|\mathbf{s}\|^3 + \frac{L_1}{2m} \|\mathbf{s}\|^2, \quad \forall \mathbf{s} \in \mathbb{R}^d.$$

Convergence Analysis

- For simplicity, we further assume that $\nabla^2 f(\mathbf{x}) \preceq L_1 \mathbf{I}$ as in [Hanzely et al.'20]

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- ▶ The additional error term is independent of d
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- ▶ Recall the Lanczos algorithm generates $\{\mathbf{v}_j\}_{j=1}^m$ and $\{\beta_{j+1}\}_{j=1}^m$:

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- Since $\{\mathbf{v}_j\}$ are **orthonormal**, we further have $\min_{j \in \{1, \dots, m\}} |\mathbf{v}_j^\top \mathbf{s}| |\mathbf{v}_{j+1}^\top \mathbf{s}| \leq \frac{1}{m} \|\mathbf{s}\|^2$

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Let $\{\mathbf{x}_k\}$ be generated by the Krylov CRN method. Then we have

$$f(\mathbf{x}_k) - f^* \leq \frac{9L_1D^2}{2mk} + \frac{9L_2D^3}{k^2}$$

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Main Result: Strongly Convex Setting

- ▶ We also consider the strongly convex setting, i.e., $\nabla^2 f(\mathbf{x}) \succeq \mu \mathbf{I}, \forall \mathbf{x} \in \mathbb{R}^d$

Theorem

Let $\{\mathbf{x}_k\}$ be generated by the Krylov CRN method. Then, the number of iterations required to reach $\delta_k := f(\mathbf{x}_k) - f(\mathbf{x}^*) \leq \epsilon$ can be upper bounded by

$$k = \mathcal{O}\left(\left(\frac{L_1}{m\mu} + 1\right) \log \frac{\delta_0}{\epsilon} + \frac{\sqrt{L_2} \delta_0^{0.25}}{\mu^{0.75}}\right)$$

- ▶ In comparison, SSCN requires $\mathcal{O}\left(\left(\frac{d-m}{m} \frac{L_1}{\mu} + \frac{d}{m}\right) \log \frac{1}{\epsilon}\right)$
- ▶ Again, when $m \ll d$, we shave a factor of d

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- ▶ Let $\mathcal{M}_m$ be the set of **monic polynomials** of degree m . Then we have

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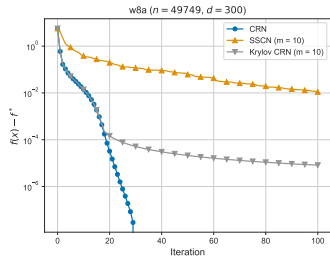
- ▶ Example II: Assume that all the eigenvalues of $\mathbf{H}$ lie within $[0, \Delta] \cup [L_1 - \Delta, L_1]$ for some $L_1 > \Delta > 0$. Then, when m is even, we have

$$\rho^{(m)}(\mathbf{H}, \mathbf{g}) \leq 2^{1/m} \sqrt{\Delta(L_1 - \Delta)}/2$$

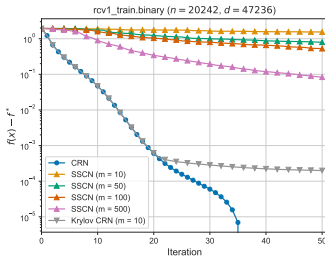
Outline

- ① Introduction
- ② The Proposed Method
- ③ Convergence Analysis
- ④ Numerical Results

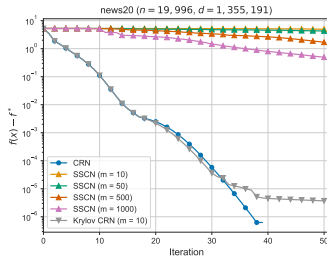
Logistic Regression Problems



(a) w8a ($d = 300$)



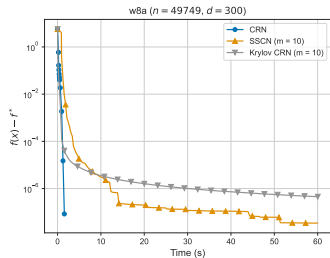
(b) rcv1 ($d = 47,236$)



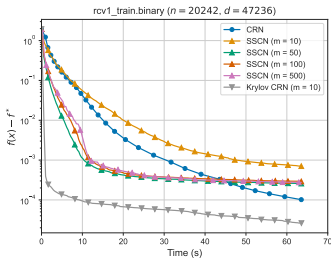
(c) news20 ($d = 1,355,191$)

- ▶ The convergence path of Krylov-CRN remains almost unchanged as d increases
- ▶ SSCN converges slower as d increases

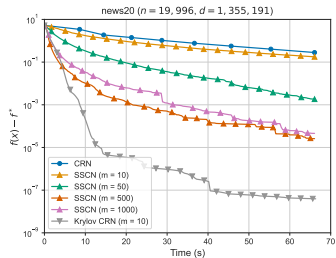
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- When d is large, Krylov CRN converges much faster than the others

Ruichen Jiang, Parameswaran Raman, Shoham Sabach, Aryan Mokhtari, Mingyi Hong, and Volkan Cevher. Krylov Cubic Regularized Newton: A Subspace Second-Order Method with Dimension-Free Convergence Rate, 2024. [arXiv: 2401.03058](https://arxiv.org/abs/2401.03058) [math.OC]

Thank you!