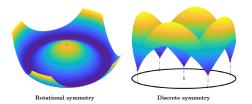
Computational Principles for High-dim Data Analysis (Lecture Seventeen)

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Nonconvex Optimization for High-Dim Problems First Order Methods

- 1 Objectives of Nonconvex Optimization
- 2 Gradient Descent and Newton's Method
- **3** First Order Methods for Nonconvex Problems

Gradient and Negative Curvature Descent (Inexact) Negative Curvature and Newton Descent (Inexact) Gradient Descent with Small Random Noise Hybrid Noisy Gradient Descent

> "Premature optimization is the root of all evil." - Donald Knuth, The Art of Computer Programming

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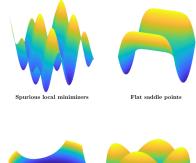
Nonconvex Optimization

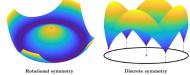
Consider the problem of minimizing a general nonlinear function:

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathsf{C}. \tag{1}$$

In the worst case, even finding a *local* minimizer can be NP-hard¹.

Nonconvex problems that arise from natural physical, geometrical, or statistical origins typically have nice structures, in terms of symmetries!





¹Some NP-complete problems in quadratic and nonlinear programming, K.G Murty and S. N. Kabadi, 1987

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Objectives

Hence typically people seek to work with relatively benign (gradient Lipschitz continuous) functions:

$$\forall \boldsymbol{x}, \boldsymbol{y} \quad \|\nabla f(\boldsymbol{y}) - \nabla f(\boldsymbol{x})\|_2 \le L_1 \|\boldsymbol{y} - \boldsymbol{x}\|_2$$
(2)

with benign objectives:

- **()** convergence to some critical point x_{\star} such that: $\nabla f(x_{\star}) = 0$;
- **2** the critical point x_{\star} is second-order stationary: $\nabla^2 f(x_{\star}) \succeq \mathbf{0}$.

Example: in general f could have irregular second-order stationary points:

Second Order Stationary Points

$$\begin{aligned} \cdot f(w) &= \frac{1}{3}(w_1^3 - 3w_1w_2^2) \\ \cdot \nabla f(w) &= \begin{bmatrix} (w_1^2 - w_2^2) \\ -2w_1w_2 \end{bmatrix} \\ \cdot \nabla^2 f(w) &= \begin{bmatrix} 2w_1 & -2w_2 \\ -2w_2 & -2w_1 \end{bmatrix} \\ \cdot \nabla f(0) &= 0, \nabla^2 f(0) = 0 \Rightarrow 0 \text{ is } SOSP \\ \cdot f([\epsilon, \epsilon]) &= -\frac{2}{3}\epsilon^3 < f(0) \end{aligned}$$

Second Order Stationary Point (SOSP)

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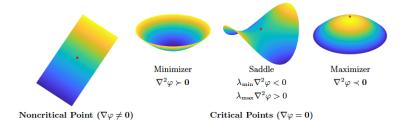
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Objectives

Hence typically people seek to work with relatively benign (gradient Lipschitz continuous) functions with benign objectives:

- **1** convergence to some critical point $m{x}_{\star}$ such that: $abla f(m{x}_{\star}) = m{0}$;
- **2** the critical point x_{\star} is second-order stationary: $\nabla^2 f(x_{\star}) \succeq \mathbf{0}$.

Example: a function φ with symmetry only has **regular** critical points:



Gradient Descent (GD)

Function class: ∇f Lipschitz continuous with constant L_1 .

First-order oracle: the gradient $\nabla f(x)$ of the function f(x).

The gradient descent iteration:

$$\boldsymbol{x}_k = \boldsymbol{x}_{k-1} - \gamma_k \nabla f(\boldsymbol{x}_{k-1}).$$
 (3)

Proposition (Convergence Rate of GD for Nonconvex Functions)

Suppose that f(x) is a (possibly nonconvex) differentiable function with ∇f Lipschitz continuous with constant L_1 . The gradient descent scheme with the step size $\gamma_k = 1/L_1$ converges to a critical point x_* . Furthermore, for the gradient norm at the best iterate $\min_{0 \le i \le k-1} \|\nabla f(x_i)\|_2 \le \epsilon_g$, the number of iterations $k = O(\epsilon_g^{-2})$.

Newton's Method (strong convex)

Function class: f strongly convex and $\nabla^2 f$ Lipschitz continuous with L_2 . **The second-order oracle**: the gradient $\nabla f(\boldsymbol{x})$ and the Hessian $\nabla^2 f(\boldsymbol{x})$. **The Newton iteration**:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \left[\nabla^2 f(\boldsymbol{x}_k)\right]^{-1} \nabla f(\boldsymbol{x}_k). \tag{4}$$

Proposition (Convergence Rate of Newton's Method)

Let f(x) be strongly convex, with $\lambda_{\min}(\nabla^2 f(x)) \ge \lambda > 0$ for all x, and assume that $\nabla^2 f$ is Lipschitz continuous with constant L_2 , and let x_* be the (unique) minimizer of f over \mathbb{R}^n . Assuming $\|x_0 - x_*\|_2 < \frac{2\lambda}{L_2}$, the iterates x_k converge to x_* , with quadratic rate.

Unfortunately, for high-dim problems, impossible to compute $\nabla^2 f$.

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Cubic Regularized Newton's Method (nonconvex) Function class: f nonconvex and $\nabla^2 f$ Lipschitz continuous with L_2 .

The second-order oracle: the gradient $\nabla f(x)$ and the Hessian $\nabla^2 f(x)$. Consider the local cubic surrogate:

$$\hat{f}(\boldsymbol{y}, \boldsymbol{x}) \doteq f(\boldsymbol{x}) + \langle \nabla f(\boldsymbol{x}), \boldsymbol{y} - \boldsymbol{x} \rangle + \frac{1}{2} (\boldsymbol{y} - \boldsymbol{x})^* \nabla^2 f(\boldsymbol{x}) (\boldsymbol{y} - \boldsymbol{x}) + \frac{L_2}{6} \| \boldsymbol{y} - \boldsymbol{x} \|_2^3.$$
 (5)

The cubic Newton iteration:

$$\boldsymbol{x}_{k+1} = \arg\min_{\boldsymbol{y}} \hat{f}(\boldsymbol{y}, \boldsymbol{x}_k).$$
(6)

Theorem (Convergence Rate of Cubic Newton's Method)

Suppose f(x) is bounded from below. Then the sequence $\{x_k\}$ generated by the cubic regularized Newton step (6) converges to a non-empty set of limit points X_* of SOS points. For $\|\nabla f(x_k)\|_2 \le \epsilon_g$, the number of iterations $k = O(\epsilon_g^{-3/2})$.

Unfortunately, for high-dim problems, impossible to compute $abla^2_{\pm}f_{\cdot, \gamma, \gamma, \gamma}$

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Gradient and Negative Curvature Descent

Function class: f nonconvex and $\nabla^2 f$ Lipschitz continuous with L_2 .

The oracle: gradient $\nabla f(x)$ and a negative eigenvector e of $\nabla^2 f(x)$.

Hybrid gradient and negative curvature descent:

• if
$$\|\nabla f(\boldsymbol{x}_k)\|_2 \ge \epsilon_g = (2L_1\epsilon)^{1/2}$$
, then $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \frac{1}{L_1}\nabla f(\boldsymbol{x}_k)$;

• else if
$$-\lambda_k(\nabla^2 f(\boldsymbol{x})) \ge \epsilon_H = \left(1.5L_2^2\epsilon\right)^{1/3}$$
, then $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \frac{2\lambda_k}{L_2}\boldsymbol{e}_k$.

Theorem (Convergence of Gradient and Negative Curvature Descent)

The above hybrid gradient and negative curvature descent scheme converges to a second-order stationary point x_* with the desired precision in function value ϵ in no more than $k = (f(x_0) - f(x_*))/\epsilon$ iterations. Or in terms of $\|\nabla f(x_k)\|_2 \le \epsilon_g$, $k = O(\epsilon_g^{-2})$.

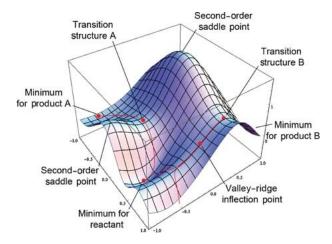
The same convergence rate as GD, but converges to an SOS point!

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Gradient and Negative Curvature Descent

An Example: potential energy surface in Chemistry.



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Compute Negative Curvature: the Power Iteration

Hessian: $H \doteq \nabla^2 f(x)$. Want to compute negative curvature direction e:

$$He = \lambda_{\min}(H)e$$
 or $Ae = \lambda_{\max}(A)e$, with $A \doteq I - L_1^{-1}H \succ 0$.

Power iteration:

$$\hat{\lambda}_{k+1} = rac{\langle oldsymbol{A}oldsymbol{x}, oldsymbol{x}
angle}{\langle oldsymbol{x}, oldsymbol{x}
angle}, \quad oldsymbol{x} = oldsymbol{A}^k oldsymbol{b},$$

where $A^i b$ can be approximated for a small t > 0 with:

$$\boldsymbol{A}\boldsymbol{b} = \left[\boldsymbol{I} - L_1^{-1}\boldsymbol{H}\right]\boldsymbol{b} \approx \boldsymbol{b} - (tL_1)^{-1} \big(\nabla f(\boldsymbol{x} + t\boldsymbol{b}) - \nabla f(\boldsymbol{x})\big).$$

Two gradient evaluations per iteration.

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Compute Negative Curvature: the Lanczos Method

The Krylov information: $\mathbf{K} \doteq \begin{bmatrix} \mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \dots, \mathbf{A}^k\mathbf{b} \end{bmatrix}$.

The Lanczos method:

$$\hat{\lambda}_{k+1} = \max_{oldsymbol{x}} rac{\langle oldsymbol{A} oldsymbol{x}, oldsymbol{x}
angle}{\langle oldsymbol{x}, oldsymbol{x}
angle}, \quad oldsymbol{x} \in \mathsf{span}(oldsymbol{K}).$$

Proposition (Convergence Rate of Lanczos)

Use the Lanczos procedure to find the largest eigenvalue of $\mathbf{I} - L_1^{-1}\mathbf{H}$ starting from a random unit vector. Then, for any $\epsilon_{\lambda} > 0$ and $\delta \in (0, 1)$, with a probability at least $1 - \delta$ the procedure outputs a unit vector \mathbf{e}' such that $(\mathbf{e}')^*\mathbf{H}\mathbf{e}' \leq \lambda_{\min}(\mathbf{H}) + \epsilon_{\lambda}$ in at most number of iterations: $\min\left\{n, \frac{\log(n/\delta^2)}{2\sqrt{2}}\sqrt{\frac{L_1}{\epsilon_{\lambda}}}\right\}.$

In terms of the first-order oracle, complexity of the inexact gradient and negative curvature descent is $k \leq O(\epsilon_g^{-2})$.

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Negative Curvature and Newton Descent

Quadratic regularized Newton:

$$s_{k} = \arg\min_{s} f(\boldsymbol{x}_{k}) + \langle \nabla f(\boldsymbol{x}_{k}), \boldsymbol{s} \rangle + \frac{1}{2} \boldsymbol{s}^{*} \nabla^{2} f(\boldsymbol{x}_{k}) \boldsymbol{s} + \frac{\lambda}{2} \|\boldsymbol{s}\|_{2}^{2} \quad (7)$$

$$= -[\nabla^{2} f(\boldsymbol{x}_{k}) + \lambda \boldsymbol{I}]^{-1} \nabla f(\boldsymbol{x}_{k}). \quad (8)$$

The Levenberg-Marquardt iteration:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \left[\nabla^2 f(\boldsymbol{x}_k) + \lambda \boldsymbol{I}\right]^{-1} \nabla f(\boldsymbol{x}_k).$$
(9)

LM is popular for solving nonlinear least squares problems.

Negative Curvature and Newton Descent

Function class: f nonconvex and $\nabla^2 f$ Lipschitz continuous with L_2 .

The oracle: gradient $\nabla f(x)$ and $\nabla^2 f(x)$ (to be approximated).

Hybrid gradient and negative curvature descent:

• if
$$-\lambda_k(\nabla^2 f(\boldsymbol{x})) \ge \epsilon_H = \left(3L_2^2\epsilon\right)^{1/3}$$
, then $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \frac{2\lambda_k}{L_2}\boldsymbol{e}_k$;

• else if
$$\|
abla f(m{x}_k)\|_2 \geq \epsilon_g = 3^{8/3} L_2^{1/3} \epsilon^{2/3}/2$$
, then $m{x}_{k+1} = m{x}_k + \gamma_k m{s}_k$.

Theorem

Assume $\{x_k\}$ are generated by the hybrid negative curvature and Newton descent. Then in at most

$$k \le \frac{f(\boldsymbol{x}_0) - f(\boldsymbol{x}_\star)}{\epsilon} \tag{10}$$

iterations, x_k will be an an approximate second-order stationary point such that $\|\nabla f(x_k)\|_2 \leq \epsilon_g, \lambda_{\min}(\nabla^2 f(x_k)) \geq -\epsilon_H.$

Conjugate Gradient Descent

Need to compute e_k and s_k without knowing $\nabla^2 f(x)$. Notice that, similar to e_k , to find s_k we need solve: $[\nabla^2 f(x_k) + \lambda I] s_k = -\nabla f(x_k)$.

A special case of the quadratic minimization problem: $\min_{\boldsymbol{x}} \|\boldsymbol{y} - \boldsymbol{A} \boldsymbol{x}\|_2^2$.

Conjugate gradient descent:² Initialize the residual r_i and descent direction d_i as: $d_0 = r_0 = y - Ax_0$. Then:

Conjugate Gradient:
$$\begin{cases} \alpha_i = \frac{r_i^* r_i}{d_i^* A d_i}, \\ \boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha_i \boldsymbol{d}_i, \\ \boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \alpha_i \boldsymbol{A} \boldsymbol{d}_i, \quad i = 0, 1, 2, \dots (11) \\ \beta_{i+1} = \frac{r_{i+1}^* r_{i+1}}{r_i^* r_i}, \\ \boldsymbol{d}_{i+1} = \boldsymbol{r}_{i+1} + \beta_{i+1} \boldsymbol{d}_i. \end{cases}$$

²An introduction to the conjugate gradient method without the agonizing pain, Jonathan Shewchuk, Technical report, Carnegie Mellon University 1994.

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Negative Curvature and Newton Descent: Complexity

Theorem (Complexity of Approximate Conjugate Gradient)

To solve As = y with $\epsilon_H I \preceq A \preceq (L_1 + 2\epsilon_H)I$, the conjugate gradient method computes an s' that satisfies

$$\left\| (\nabla^2 f(\boldsymbol{x}_k) + 2\epsilon_H) \boldsymbol{s}_k + \nabla f(\boldsymbol{x}_k) \right\|_2 \le \frac{1}{2} \epsilon_H \|\boldsymbol{s}_k\|_2$$

in at most $O(\epsilon_H^{-1/2} \log(\frac{1}{\epsilon_H}))$ iterations.

With the first-order oracle, complexity of the inexact negative curvature and newton descent achieves the best known rate: $k < O(\epsilon_a^{-7/4})$.

Gradient Descent with Small Random Noise Function class: f nonconvex and $\nabla^2 f$ Lipschitz continuous with L_2 . The oracle: gradient $\nabla f(x)$ and small random noise.

The Langevin dynamics with noisy gradient flow:

$$\dot{\boldsymbol{x}}(t) = -\frac{1}{2}\nabla f(\boldsymbol{x}(t)) + \sqrt{\lambda}\boldsymbol{n}(t), \qquad (12)$$

Probability density of x converges to the **Gibbs measure**:

$$p^{\lambda}(\boldsymbol{x}) = C^{\lambda} \exp\left(-\frac{1}{\lambda}f(\boldsymbol{x})\right).$$
(13)

Lemma (Laplace's Method: Scalar Case)

Suppose f(x) is a twice continuously differentiable function with a unique maximizer x_0 and $f''(x_0) < 0$. Then we have

$$\lim_{\lambda \to 0} \int e^{\frac{1}{\lambda}f(x)} dx = e^{\frac{1}{\lambda}f(x_0)} \sqrt{\frac{2\pi\lambda}{-f''(x_0)}} \propto \int e^{\frac{1}{\lambda}f(x)} \delta(x-x_0) dx.$$
(14)

The Laplace Method

Theorem (Laplace Method: Multivariate and Multiple Global Minimizers)

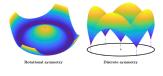
Let f(x) be a function with at least quadratic growth as $x \to \infty$. Suppose f(x) has multiple global non-degenerate minimizers at $x_{\star}^1, \ldots, x_{\star}^N$ and they are all non-degenerate. Then in the limit $\lambda \downarrow 0$, the density $p^{\lambda}(x)$ converges to

$$p^{0}(\boldsymbol{x}) = \frac{\sum_{i=1}^{N} a_{i} \delta(\boldsymbol{x} - \boldsymbol{x}_{\star}^{i})}{\sum_{i=1}^{N} a_{i}}, \quad \text{with} \quad a_{i} = \det[\boldsymbol{H}(\boldsymbol{x}_{\star}^{i})]^{-1/2}, \tag{15}$$

where $H(x) = \nabla^2 f(x)$ is the Hessian of the function f(x).

When all global minimizers make a continuous submanifold \mathcal{M} , $p^{\lambda}(\boldsymbol{x})$ converges to a density on \mathcal{M} given by:

$$p^0(oldsymbol{x}) = rac{\det[oldsymbol{H}(oldsymbol{x})]^{-1/2}}{\int_{\mathcal{M}} \det[oldsymbol{H}(oldsymbol{y})]^{-1/2} doldsymbol{y}}, \quad oldsymbol{x} \in \mathcal{M}.$$



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Noisy Gradient with Langevin Monte Carlo

Function class: ∇f Lipschitz continuous with constant L_1 . **First-order oracle**: the gradient $\nabla f(x)$ and small noise n.

Langevin Monte Carlo:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \frac{1}{L_1} \nabla f(\boldsymbol{x}_k) + \sqrt{2\lambda/L_1} \boldsymbol{n}_k.$$
 (16)

Proposition (Noisy Gradient Descent)

Considering the above noisy gradient descent scheme (16), if $\|\nabla f(\boldsymbol{x}_k)\|_2 \ge (2L_1\epsilon)^{1/2}$, then we have

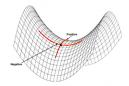
$$\mathbb{E}[f(\boldsymbol{x}_{k+1}) \mid \boldsymbol{x}_k] \le f(\boldsymbol{x}_k) - \epsilon + \lambda.$$
(17)

Descent when $\|\nabla f(\boldsymbol{x}_k)\|_2 > (2L_1\lambda)^{1/2}$; explore stability otherwise.

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Effect of Noisy Gradient around a Saddle Point

Consider a standard quadratic function: $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^*\boldsymbol{H}\boldsymbol{x}$ for a constant $\boldsymbol{H} \in \mathbb{R}^{n \times n}$, with the smallest eigenvalue $\lambda_{\min} < 0$, and the Lipschitz constant $L_1 = \max_i |\lambda_i(\boldsymbol{H})|$.



The Langevin dynamics becomes:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \frac{1}{L_1} \nabla f(\boldsymbol{x}_k) + \sqrt{2\lambda/L_1} \boldsymbol{n}_k$$
$$= \underbrace{(\boldsymbol{I} - L_1^{-1} \boldsymbol{H})}_{\boldsymbol{A}} \boldsymbol{x}_k + \underbrace{\sqrt{2\lambda/L_1}}_{\boldsymbol{b}} \boldsymbol{n}_k.$$
(18)

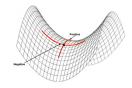
This is **an unstable linear dynamic system** with random noise as the input:

$$\boldsymbol{x}_{k+1} = \boldsymbol{A}\boldsymbol{x}_k + b\,\boldsymbol{n}_k. \tag{19}$$

Escaping Saddle Point

Therefore, the accumulated dynamics:

$$x_{k+1} = A^{k+1}x_0 + b\sum_{i=0}^k A^{k-i}n_i.$$
 (20)



 $A^{k+1}x_0$ and $A^{k-i}n_i$ are **powers** of the matrix A applied to random vectors (assuming x_0 random too).

Question: which direction survives in power iteration?

Proposition (Escaping Saddle Point via Noisy Gradient Descent)

Consider the noisy gradient descent via the Langevin dynamics (18) for the function $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^*\boldsymbol{H}\boldsymbol{x}$, starting from $\boldsymbol{x}_0 \sim \mathcal{N}(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$. Then after $k \geq \frac{\log n - \log(|\lambda_{\min}|/L_1)}{2\log(1+|\lambda_{\min}|/L_1)}$ steps, we have

$$\mathbb{E}[f(\boldsymbol{x}_{k+1}) - f(\boldsymbol{x}_0)] \le -\lambda.$$
(21)

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Hybrid Noisy Gradient Descent

Function class: f nonconvex and $\nabla^2 f$ Lipschitz continuous with L_2 .

The oracle: gradient $\nabla f(\boldsymbol{x})$ and small noise \boldsymbol{n} .

Hybrid noisy gradient descent:

- if $\|\nabla f(\boldsymbol{x}_k)\|_2 \ge \epsilon_g$, then $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k \frac{1}{L_1} \nabla f(\boldsymbol{x}_k);$
- else $x_k^0 = x_k$, and negative curvature descent with noisy gradients: for $i = 0, 1, 2, ..., k_{\max} = O(\log n)$

$$oldsymbol{x}_k^{i+1} = oldsymbol{x}_k^i - rac{1}{L_1}
abla f(oldsymbol{x}_k^i) + \sqrt{2\epsilon/L_1} oldsymbol{n}^i,$$

where $\boldsymbol{n}^i \sim \mathcal{N}(0, \boldsymbol{I})$.

Complexity: To guarantee $\|\nabla f(x)\| \le \epsilon_g$, the number of total gradient evaluations needed is $O(\epsilon_q^{-2})$, up to a $\log(n)$ factor.³

³Perturbed accelerated gradient descent reduces to $O(\epsilon_q^{-7/4})$.

Summary

Table: Oracles and complexities (up to log factors) of different optimization methods. "Stat. Point" stands for the type of stationary point x_{\star} to which the method guarantees to converge. Complexity is measured in terms of the number of oracles accessed before attaining a prescribed accuracy $\|\nabla f(x_{\star})\| \leq \epsilon_q$.

Method	Oracle	Stat. Point	Complexity
Vanilla gradient descent	first-order	first-order	$O(\epsilon_g^{-2})$
Cubic Regularized Newton	second-order	second-order	$O(\epsilon_g^{-1.5})$
Gradient/negative curvature	first-order	second-order	$O(\epsilon_g^{-2})$
Negative curvature/Newton	first-order	second-order	$O(\epsilon_g^{-1.75})$
Hybrid noisy gradient	first-order	second-order	$O(\epsilon_g^{-2})$
Perturbed accelerated gradient	first-order	second-order	$O(\epsilon_g^{-1.75})$

Assignments

- Reading: Section 9.1 9.5 of Chapter 9.
- Programming Homework #3.

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