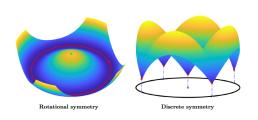
Computational Principles for High-dim Data Analysis

(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 (Perturbed) Gradient Descent

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

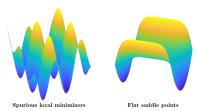
Nonconvex Optimization

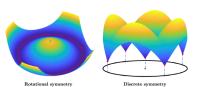
Consider the problem of minimizing a general nonlinear function:

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

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

Objectives

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

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

with benign objectives:

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

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

Second Order Stationary Points

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

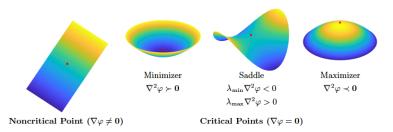
Second Order Stationary Point (SOSP)

Objectives

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

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

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).

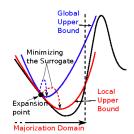
The gradient descent iteration:

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

$$x_k := \underset{x}{\operatorname{arg min}} \left\{ f(x_{k-1}) + \langle \nabla f(x_{k-1}), x - x_{k-1} \rangle + \frac{L_1}{2} ||x - x_{k-1}||_2^2 \right\}.$$

Proposition (Convergence Rate of GD for Nonconvex Functions)

The gradient descent scheme with the step size $\gamma_k = 1/L_1$ converges to a critical point \boldsymbol{x}_{\star} . Furthermore, for the gradient norm at the best iterate $\min_{0 \leq i \leq k-1} \|\nabla f(\boldsymbol{x}_i)\|_2 \leq \epsilon_g$, 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 $\nabla f(x)$ and the Hessian $\nabla^2 f(x)$.

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

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

Cubic Regularized Newton's Method (nonconvex)

Function class: f nonconvex and $\nabla f/\nabla^2 f$ Lips. continuous with L_1/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:

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

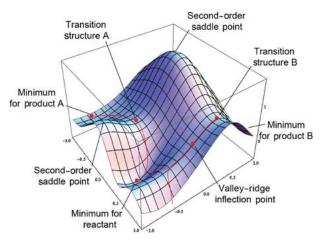
Theorem (Convergence Rate of Cubic Newton's Method)

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_\star of SOS points. For $\|\nabla f(x_k)\|_2 \le \epsilon_g$, the number of iterations $k = O(\epsilon_q^{-3/2})$.

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

Gradient and Negative Curvature Descent

An Intuitive Example: potential energy surface in Chemistry.



Gradient and Negative Curvature Descent

Function class: f nonconvex and $\nabla f/\nabla^2 f$ Lips. continuous with L_1/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_{\star} with the desired precision in function value ϵ in no more than $k = (f(x_0) - f(x_{\star}))/\epsilon$ 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!

Compute Negative Curvature: the Power Iteration

Want to compute negative curvature direction e without Hessian $\mathbf{H} \doteq \nabla^2 f(\mathbf{x})$:

$$oldsymbol{H}oldsymbol{e}=\lambda_{\min}(oldsymbol{H})oldsymbol{e} \quad ext{or} \quad oldsymbol{A}oldsymbol{e}=\lambda_{\max}(oldsymbol{A})oldsymbol{e},$$

with
$$\mathbf{A} \doteq \mathbf{I} - L_1^{-1}\mathbf{H} \succ \mathbf{0}$$
.

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^ib can be approximated for a small t > 0 with:

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

Two gradient evaluations per iteration.

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Compute Negative Curvature: the Lanczos Method

The Krylov information:

$$K \doteq [b, Ab, A^2b, \dots, A^kb].$$

The Lanczos method:

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

Proposition (Convergence Rate of Lanczos)

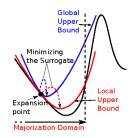
Use the Lanczos procedure to find the largest eigenvalue of $\mathbf{I} - L_1^{-1}\mathbf{H}$ starting from a random unit vector. Then, for any $\epsilon_{\lambda} > 0$ and $\delta \in (0,1)$, with a probability at least $1-\delta$ the procedure outputs a unit vector \mathbf{e}' such that $(\mathbf{e}')^*\mathbf{H}\mathbf{e}' \leq \lambda_{\min}(\mathbf{H}) + \epsilon_{\lambda}$ 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 $k \leq O(\epsilon_q^{-2})$.

Negative Curvature and Newton Descent

Consider a nonconvex program:

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}).$$



Quadratic regularized Newton:

$$s_k = \underset{s}{\operatorname{arg min}} f(\boldsymbol{x}_k) + \langle \nabla f(\boldsymbol{x}_k), \boldsymbol{s} \rangle + \frac{1}{2} \boldsymbol{s}^* \nabla^2 f(\boldsymbol{x}_k) \boldsymbol{s} + \frac{\lambda}{2} \|\boldsymbol{s}\|_2^2 \quad (7)$$
$$= -[\nabla^2 f(\boldsymbol{x}_k) + \lambda \boldsymbol{I}]^{-1} \nabla f(\boldsymbol{x}_k). \quad (8)$$

The Levenberg-Marquardt iteration:

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

LM is very popular for solving nonlinear least squares problems.

Negative Curvature and Newton Descent

Function class: f nonconvex and $\nabla f/\nabla^2 f$ Lips. continuous with L_1/L_2 .

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

Hybrid curvature and Newton descent (why flip order?):

- if $-\lambda_k(\nabla^2 f(x)) \ge \epsilon_H = \left(3L_2^2\epsilon\right)^{1/3}$, then $x_{k+1} = x_k + \frac{2\lambda_k}{L_2}e_k$;
- else if $\|\nabla f(x_k)\|_2 \ge \epsilon_g = 3^{8/3} L_2^{1/3} \epsilon^{2/3} / 2$, then $x_{k+1} = x_k + \gamma_k s_k$.

Theorem

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

$$k \le \frac{f(x_0) - f(x_\star)}{\epsilon} \tag{10}$$

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

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: $\underbrace{\left[\nabla^2 f(x_k) + \lambda I\right]}_{:} s_k = \underbrace{-\nabla f(x_k)}_{:}$.

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

Conjugate gradient descent:² Initialize the residual r_i and descent direction d_i as: $d_0 = r_0 = y - Ax_0$. Then for i = 0, 1, 2, ...:

$$\text{Conjugate Gradient:} \left\{ \begin{array}{rcl} \alpha_i & = & \frac{\boldsymbol{r}_i^* \boldsymbol{r}_i}{\boldsymbol{d}_i^* \boldsymbol{A} \boldsymbol{d}_i}, \\ \boldsymbol{x}_{i+1} & = & \boldsymbol{x}_i + \alpha_i \boldsymbol{d}_i, \\ \boldsymbol{r}_{i+1} & = & \boldsymbol{r}_i - \alpha_i \boldsymbol{A} \boldsymbol{d}_i, \\ \beta_{i+1} & = & \frac{\boldsymbol{r}_{i+1}^* \boldsymbol{r}_{i+1}}{\boldsymbol{r}_i^* \boldsymbol{r}_i}, \\ \boldsymbol{d}_{i+1} & = & \boldsymbol{r}_{i+1} + \beta_{i+1} \boldsymbol{d}_i. \end{array} \right.$$

Contours

— Conjugate Gradent
— Steepest Descent

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

Negative Curvature and Newton Descent: Complexity

Theorem (Complexity of Approximate Conjugate Gradient)

To solve As = y with $\epsilon_H I \leq A \leq (L_1 + 2\epsilon_H)I$, 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: $k \leq O(\epsilon_g^{-7/4})$.

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Gradient Descent with Small Random Noise

Function class: f nonconvex and $\nabla f/\nabla^2 f$ Lips. continuous with L_1/L_2 .

The oracle: gradient $\nabla f(x)$ and small random noise.

The **Langevin dynamics** with noisy gradient flow:

$$\dot{\boldsymbol{x}}(t) = -\frac{1}{2}\nabla f(\boldsymbol{x}(t)) + \sqrt{\lambda}\boldsymbol{n}(t), \tag{11}$$

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

$$p^{\lambda}(\boldsymbol{x}) = C^{\lambda} \exp\left(-\frac{1}{\lambda}f(\boldsymbol{x})\right).$$
 (12)

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

$$\lim_{\lambda \to 0} \int e^{\frac{1}{\lambda}f(x)} dx = e^{\frac{1}{\lambda}f(x_0)} \sqrt{\frac{2\pi\lambda}{-f''(x_0)}} \propto \int e^{\frac{1}{\lambda}f(x)} \delta(x - x_0) dx. \quad (13)$$

The Laplace Method

Theorem (Laplace Method: Multivariate and Multiple Global Minimizers)

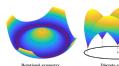
Let f(x) be a function with at least quadratic growth as $x \to \infty$. Suppose f(x) has multiple global non-degenerate minimizers at $x^1_\star, \ldots, x^N_\star$ and they are all non-degenerate. Then in the limit $\lambda \downarrow 0$, the density $p^\lambda(x)$ converges to

$$p^{0}(\mathbf{x}) = \frac{\sum_{i=1}^{N} a_{i} \delta(\mathbf{x} - \mathbf{x}_{\star}^{i})}{\sum_{i=1}^{N} a_{i}}, \quad \text{with} \quad a_{i} = \det[\mathbf{H}(\mathbf{x}_{\star}^{i})]^{-1/2}, \tag{14}$$

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} , $p^{\lambda}(x)$ converges to a density on \mathcal{M} given by:

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



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:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \frac{1}{L_1} \nabla f(\boldsymbol{x}_k) + \sqrt{2\lambda/L_1} \boldsymbol{n}_k. \tag{15}$$

Proposition (Noisy Gradient Descent)

Considering the above noisy gradient descent scheme (15), if $\|\nabla f(x_k)\|_2 \geq (2L_1\epsilon)^{1/2}$, then we have

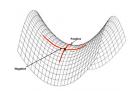
$$\mathbb{E}[f(\boldsymbol{x}_{k+1}) \mid \boldsymbol{x}_k] \le f(\boldsymbol{x}_k) - \epsilon + \lambda. \tag{16}$$

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



The Langevin dynamics becomes:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{1}{L_1} \nabla f(\mathbf{x}_k) + \sqrt{2\lambda/L_1} \mathbf{n}_k$$
$$= \underbrace{(\mathbf{I} - L_1^{-1} \mathbf{H})}_{\mathbf{A}} \mathbf{x}_k + \underbrace{\sqrt{2\lambda/L_1}}_{\mathbf{b}} \mathbf{n}_k. \tag{17}$$

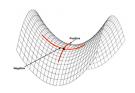
Since $\lambda_{\max}(A) = 1 - \lambda_{\min}(H)/L_1 > 1$, this is an unstable linear dynamic system with random noise as the input:

$$\boldsymbol{x}_{k+1} = \boldsymbol{A}\boldsymbol{x}_k + b\,\boldsymbol{n}_k. \tag{18}$$

Escaping Saddle Point

Therefore, the accumulated dynamics:

$$x_{k+1} = A^{k+1}x_0 + b\sum_{i=0}^{k} A^{k-i}n_i.$$
 (19)



 $m{A}^{k+1}m{x}_0$ and $m{A}^{k-i}m{n}_i$ are **powers** of the matrix $m{A}$ applied to random vectors (assuming $m{x}_0$ 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 (17) for the function $f(x) = \frac{1}{2}x^*Hx$, starting from $x_0 \sim \mathcal{N}(\mathbf{0}, \sigma^2 I)$. Then after $k \geq \frac{\log n - \log(|\lambda_{\min}|/L_1)}{2\log(1+|\lambda_{\min}|/L_1)}$ steps, we have

$$\mathbb{E}[f(\boldsymbol{x}_{k+1}) - f(\boldsymbol{x}_0)] \le -\lambda. \tag{20}$$

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Hybrid Noisy Gradient Descent

Function class: f nonconvex and $\nabla f/\nabla^2 f$ Lips. continuous with L_1/L_2 .

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

Hybrid noisy gradient descent:

- if $\|\nabla f(\boldsymbol{x}_k)\|_2 \geq \epsilon_g$, 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 $i=0,1,2,\ldots,k_{\max}=O(\log n)$

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

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 $O(\epsilon_{g^{-}}^{-7/4})$.

Summary

Table: Oracles and complexities (up to log factors) of different optimization methods. Complexity is measured in terms of the number of oracles accessed before attaining a prescribed accuracy $\|\nabla f(\boldsymbol{x}_{\star})\| \leq \epsilon_g$.

Methods	Oracles	Stat. Points	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	$O(\epsilon_g^{-1.75})$

The (probably only) two fundamental ideas for first-order optimization: **Gradient Descent and Acceleration.**

Power Iteration for Inexact Newton Descent.

Assignments

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