

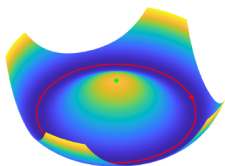
# Computational Principles for High-dim Data Analysis

## (Lecture Eighteen)

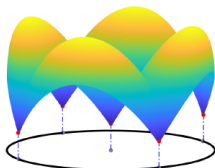
**Yi Ma**

EECS Department, UC Berkeley

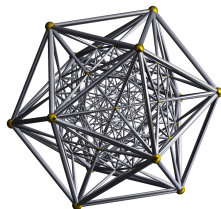
November 2, 2021



Rotational symmetry



Discrete symmetry



# Nonconvex Optimization for High-Dim Problems

## Power Iteration and Fixed Point

- 1 Power Iteration is Everywhere
- 2 Singular Vectors as Fixed Point
- 3 Complete Dictionary Learning as Fixed Point
- 4 Generalized Power Iteration as Fixed Point
- 5 Fixed Point of a Contracting Mapping

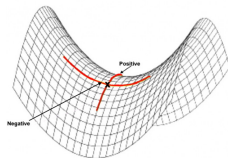
*“Truth is ever to be found in the simplicity, and not in the multiplicity and confusion of things.”*

– Isaac Newton

# Negative Curvature and Newton Descent

Consider a nonconvex program:

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



**Negative curvature descent:** compute  $\mathbf{e}_k$  satisfying  $\mathbf{A}\mathbf{e}_k = \lambda_{\max}(\mathbf{A})\mathbf{e}_k$  with  $\mathbf{A} \doteq \mathbf{I} - L_1^{-1}\nabla^2 f(\mathbf{x}_k) \succ \mathbf{0}$  by power iteration:

$$\hat{\lambda}_{i+1} = \frac{\langle \mathbf{A}\mathbf{x}, \mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}, \quad \mathbf{x} = \mathbf{A}^i \mathbf{b}, \quad i = 1, 2, \dots \quad (1)$$

**Newton descent:** compute descent  $\mathbf{s}_k$  from

$$\mathbf{s}_k = \arg \min_{\mathbf{s}} f(\mathbf{x}_k) + \langle \nabla f(\mathbf{x}_k), \mathbf{s} \rangle + \frac{1}{2} \mathbf{s}^* \nabla^2 f(\mathbf{x}_k) \mathbf{s} + \frac{\lambda}{2} \|\mathbf{s}\|_2^2 \quad (2)$$

$$= -[\nabla^2 f(\mathbf{x}_k) + \lambda \mathbf{I}]^{-1} \nabla f(\mathbf{x}_k). \quad (3)$$

## 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  $\nabla f(\mathbf{x})$  and  $\nabla^2 f(\mathbf{x})$  (to be approximated).

**Hybrid gradient and negative curvature descent:**

- if  $-\lambda_k(\nabla^2 f(\mathbf{x})) \geq \epsilon_H = (3L_2^2\epsilon)^{1/3}$ , then  $\mathbf{x}_{k+1} = \mathbf{x}_k + \frac{2\lambda_k}{L_2} \mathbf{e}_k$ ;
- else if  $\|\nabla f(\mathbf{x}_k)\|_2 \geq \epsilon_g = 3^{8/3} L_2^{1/3} \epsilon^{2/3} / 2$ , then  $\mathbf{x}_{k+1} = \mathbf{x}_k + \gamma_k \mathbf{s}_k$ .

### Theorem

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

$$k \leq \frac{f(\mathbf{x}_0) - f(\mathbf{x}_*)}{\epsilon} \quad (4)$$

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

# Compute Negative Curvature: the Power Iteration

Need to compute negative curvature direction  $e_k$  without Hessian:

$$H \doteq \nabla^2 f(x):$$

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

**Power iteration:**

$$\hat{\lambda}_{i+1} = \frac{\langle Ax, x \rangle}{\langle x, x \rangle}, \quad x = A^i b, \quad i = 1, 2, \dots,$$

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

$$Ab = [I - L_1^{-1}H] b \approx b - (tL_1)^{-1}(\nabla f(x + tb) - \nabla f(x)).$$

**Two gradient evaluations per power iteration.**

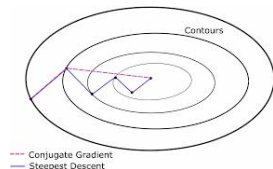
# Conjugate Gradient Descent

Need to compute  $s_k$  without knowing  $\mathbf{H} = \nabla^2 f(\mathbf{x})$ . Notice that, similar to  $e_k$ , to find  $s_k$  we need solve:  $\underbrace{[\mathbf{H} + \lambda \mathbf{I}]}_{\mathbf{A}} \mathbf{s}_k = \underbrace{-\nabla f(\mathbf{x}_k)}_{\mathbf{y}}$ .

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

**Conjugate gradient descent:**<sup>1</sup> Initialize the residual  $\mathbf{r}_i$  and descent direction  $\mathbf{d}_i$  as:  $\mathbf{d}_0 = \mathbf{r}_0 = \mathbf{y} - \mathbf{A}\mathbf{x}_0$ . Then for  $i = 0, 1, 2, \dots$ :

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



<sup>1</sup>An introduction to the conjugate gradient method without the agonizing pain, Jonathan Shewchuk, Technical report, Carnegie Mellon University, 1994.

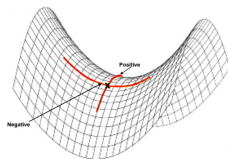
# Effect of Noisy Gradient around a Saddle Point

Consider a standard quadratic function:

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^* \mathbf{H} \mathbf{x} \text{ for a constant } \mathbf{H} \in \mathbb{R}^{n \times n},$$

with the smallest eigenvalue  $\lambda_{\min} < 0$ ,

and the Lipschitz constant  $L_1 = \max_i |\lambda_i(\mathbf{H})|$ .



The Langevin dynamics is:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k - \frac{1}{L_1} \nabla f(\mathbf{x}_k) + \sqrt{2\lambda/L_1} \mathbf{n}_k \\ &= \underbrace{(\mathbf{I} - L_1^{-1} \mathbf{H})}_{\mathbf{A}} \mathbf{x}_k + \underbrace{\sqrt{2\lambda/L_1}}_b \mathbf{n}_k. \end{aligned} \quad (5)$$

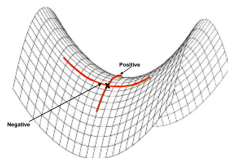
Since  $\lambda_{\max}(\mathbf{A}) = 1 - \lambda_{\min}(\mathbf{H})/L_1 > 1$ , this is **an unstable linear dynamic system** with random noise as the input:

$$\mathbf{x}_{k+1} = \mathbf{A} \mathbf{x}_k + b \mathbf{n}_k. \quad (6)$$

# Escaping Saddle Point

Therefore, the accumulated dynamics:

$$\mathbf{x}_{k+1} = \mathbf{A}^{k+1} \mathbf{x}_0 + b \sum_{i=0}^k \mathbf{A}^{k-i} \mathbf{n}_i. \quad (7)$$



$\mathbf{A}^{k+1} \mathbf{x}_0$  and  $\mathbf{A}^{k-i} \mathbf{n}_i$  are **powers** of the matrix  $\mathbf{A}$  applied to random vectors (assuming  $\mathbf{x}_0$  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 (5) for the function  $f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^* \mathbf{H} \mathbf{x}$ , starting from  $\mathbf{x}_0 \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ . Then after  $k \geq \frac{\log n - \log(|\lambda_{\min}|/L_1)}{2 \log(1 + |\lambda_{\min}|/L_1)}$  steps, we have

$$\mathbb{E}[f(\mathbf{x}_{k+1}) - f(\mathbf{x}_0)] \leq -\lambda. \quad (8)$$



# Power Iteration and Fixed-Point Style Algorithms

- **PCA**

- Optimization:

$$\max_{w \in \mathbb{S}^{n-1}} \varphi(w) \doteq \frac{1}{2} \|w^* Y\|_2^2$$

- Algorithm:

$$w_{t+1} = \mathcal{P}_{\mathbb{S}^{n-1}} [\nabla_w \varphi(w_t)] = \frac{Y Y^* w_t}{\|Y Y^* w_t\|_2}$$

- **ICA**

- Optimization:

$$\max_{w \in \mathbb{S}^{n-1}} \psi(w) \doteq \frac{1}{4} \text{kurt}[w^* y] = \frac{1}{4} \mathbb{E}[w^* y]^4 - \frac{3}{4} \|w\|_2^4$$

- Algorithm:

$$w_{t+1} = \mathcal{P}_{\mathbb{S}^{n-1}} [\nabla_w \psi(w_t)] = \frac{\mathbb{E}[y(y^* w_t)^3] - 3 \|w_t\|_2^2 w_t}{\|\mathbb{E}[y(y^* w_t)^3] - 3 \|w_t\|_2^2 w_t\|_2}$$

- **DL**

- Optimization:

$$\max_{W \in \text{St}(k, n; \mathbb{R})} \phi(W) \doteq \frac{1}{4} \|W^* Y\|_4^4$$

- Algorithm:

$$W_{t+1} = \mathcal{P}_{\text{St}(k, n; \mathbb{R})} [\nabla_W \phi(W_t)] = U_t V_t^*,$$

where  $U_t \Sigma_t V_t^* = \text{SVD}[Y(Y^* W)^{\circ 3}]$ .

# Singular Vectors via Nonconvex Optimization

To compute a singular vector of  $\mathbf{Y}$ , say  $\mathbf{u}_1$ , solve the eigenvector of  $\mathbf{\Gamma} \doteq \mathbf{Y}\mathbf{Y}^*$ :

$$\min \varphi(\mathbf{q}) \equiv -\frac{1}{2}\mathbf{q}^*\mathbf{\Gamma}\mathbf{q} \quad \text{s.t.} \quad \|\mathbf{q}\|_2^2 = 1 \quad (9)$$

Consider the Lagrangian formulation:

$$\mathcal{L}(\mathbf{q}, \lambda) = \varphi(\mathbf{q}) + \lambda(\|\mathbf{q}\|_2^2 - 1). \quad (10)$$

From the optimality condition  $\nabla_{\mathbf{q}}\mathcal{L}(\mathbf{q}, \lambda) = 0$ :

$$\nabla\varphi(\mathbf{q}) = \mathbf{\Gamma}\mathbf{q} = 2\lambda\mathbf{q} \quad \text{for some } \lambda. \quad (11)$$

*The critical points are precisely the eigenvectors  $\pm\mathbf{u}_i$  of  $\mathbf{\Gamma}$ :*

**All  $\pm\mathbf{u}_i$  are unstable critical points of  $\varphi$  over  $\mathbb{S}^{n-1}$  except  $\pm\mathbf{u}_1$ !**

## Fixed Point Interpretation and Power Iteration

Any critical point, including the optimal solution, is a “fixed point” to the following equation:

$$\mathbf{q} = \mathcal{P}_{\mathbb{S}^{n-1}}(\mathbf{\Gamma}\mathbf{q}) = \frac{\mathbf{\Gamma}\mathbf{q}}{\|\mathbf{\Gamma}\mathbf{q}\|_2}, \quad (12)$$

where  $\mathcal{P}_{\mathbb{S}^{n-1}}$  means projection onto the sphere  $\mathbb{S}^{n-1}$ . The map:

$$g(\cdot) \doteq \mathcal{P}_{\mathbb{S}^{n-1}}[\mathbf{\Gamma}(\cdot)] : \mathbb{S}^{n-1} \rightarrow \mathbb{S}^{n-1}$$

is actually a **contracting map** from  $\mathbb{S}^{n-1}$  to  $\mathbb{S}^{n-1}$ :

$$d(g(\mathbf{q}), g(\mathbf{p})) \leq \rho \cdot d(\mathbf{q}, \mathbf{p})$$

for some  $0 < \rho \leq \lambda_2/\lambda_1 < 1$  and  $d(\cdot, \cdot)$  a natural distance on the sphere. Hence the power iteration:

$$\mathbf{q}_{k+1} = g(\mathbf{q}_k) = \frac{\mathbf{\Gamma}\mathbf{q}_k}{\|\mathbf{\Gamma}\mathbf{q}_k\|_2} \in \mathbb{S}^{n-1}. \quad (13)$$

# Contracting Map

## Proposition

Let  $\Gamma \in \mathbb{R}^{n \times n}$  be a matrix with left eigenvalue-eigenvector pairs  $(\lambda_1, \mathbf{u}_1), \dots, (\lambda_n, \mathbf{u}_n)$  such that  $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n$ . Then the power iteration is contracting under the metric:  $d(\mathbf{x}, \mathbf{y}) \doteq \left\| \frac{\mathbf{x}}{\langle \mathbf{x}, \mathbf{u}_1 \rangle} - \frac{\mathbf{y}}{\langle \mathbf{y}, \mathbf{u}_1 \rangle} \right\|_2$  with contraction constant  $\lambda_2/\lambda_1$  for all  $\mathbf{x}, \mathbf{y} \perp \mathbf{u}_1$ :  $d(g(\mathbf{x}), g(\mathbf{y})) \leq \frac{\lambda_2}{\lambda_1} d(\mathbf{x}, \mathbf{y})$ .

**Proof.**  $\forall \mathbf{x}$ , we have  $\langle \Gamma \mathbf{x}, \mathbf{u}_1 \rangle = \langle \mathbf{x}, \Gamma^* \mathbf{u}_1 \rangle = \lambda_1 \langle \mathbf{x}, \mathbf{u}_1 \rangle$ . So we have:

$$\begin{aligned} d(g(\mathbf{x}), g(\mathbf{y})) &= \left\| \frac{\Gamma \mathbf{x}}{\langle \Gamma \mathbf{x}, \mathbf{u}_1 \rangle} - \frac{\Gamma \mathbf{y}}{\langle \Gamma \mathbf{y}, \mathbf{u}_1 \rangle} \right\|_2 \\ &= \frac{1}{\lambda_1} \left\| \Gamma \left( \frac{\mathbf{x}}{\langle \mathbf{x}, \mathbf{u}_1 \rangle} - \frac{\mathbf{y}}{\langle \mathbf{y}, \mathbf{u}_1 \rangle} \right) \right\|_2 \\ &\leq \frac{\lambda_2}{\lambda_1} \left\| \frac{\mathbf{x}}{\langle \mathbf{x}, \mathbf{u}_1 \rangle} - \frac{\mathbf{y}}{\langle \mathbf{y}, \mathbf{u}_1 \rangle} \right\|_2 = \frac{\lambda_2}{\lambda_1} d(\mathbf{x}, \mathbf{y}). \end{aligned}$$



The sequence  $q_k$  converges linearly to a unique fixed point  $q_* = \mathbf{u}_1$ .

# Complete Dictionary Learning

Given a data matrix  $\mathbf{Y} = \mathbf{D}_o \mathbf{X}_o$  where  $\mathbf{D}_o$  is orthogonal and  $\mathbf{X}_o$  is sparse, try to solve the following optimization problem:

$$\min_{\mathbf{A}} \psi(\mathbf{A}) \equiv -\frac{1}{4} \|\mathbf{A}\mathbf{Y}\|_4^4, \quad \text{subject to} \quad \mathbf{A}^* \mathbf{A} = \mathbf{I}. \quad (14)$$

Consider the Lagrangian:

$$\mathcal{L}(\mathbf{A}, \mathbf{\Lambda}) \doteq -\frac{1}{4} \|\mathbf{A}\mathbf{Y}\|_4^4 + \langle \mathbf{\Lambda}, \mathbf{A}^* \mathbf{A} - \mathbf{I} \rangle. \quad (15)$$

This gives the necessary condition  $\nabla_{\mathbf{A}} \mathcal{L}(\mathbf{A}, \mathbf{\Lambda}) = \mathbf{0}$ :

$$-\nabla_{\mathbf{A}} \psi(\mathbf{A}) = (\mathbf{A}\mathbf{Y})^{\circ 3} \mathbf{Y}^* = \mathbf{A}\mathbf{S}, \quad (16)$$

for a symmetric matrix  $\mathbf{S} = (\mathbf{\Lambda} + \mathbf{\Lambda}^*)$  (of Lagrange multipliers).

## Fixed Point Interpretation

For an orthogonal  $\mathbf{A}$  and symmetric  $\mathbf{S}$ , we have:  $\mathcal{P}_{\mathbf{O}(n)}[\mathbf{A}\mathbf{S}] = \mathbf{A}$ . (Why?)

By projecting both sides of (16) onto the orthogonal group  $\mathbf{O}(n)$ :

$$\mathbf{A} = \mathcal{P}_{\mathbf{O}(n)}[(\mathbf{A}\mathbf{Y})^{\circ 3}\mathbf{Y}^*]. \quad (17)$$

Consider the map from  $\mathbf{O}(n)$  to  $\mathbf{O}(n)$ :

$$g(\cdot) \doteq \mathcal{P}_{\mathbf{O}(n)}[((\cdot)\mathbf{Y})^{\circ 3}\mathbf{Y}^*] : \mathbf{O}(n) \rightarrow \mathbf{O}(n)$$

The optimal solutions  $\mathbf{A}_\star$  is a “fixed point” of the map  $g(\cdot)$ . This gives the *matching, stretching, and projection* algorithm for dictionary learning:

$$\mathbf{A}_{k+1} = \mathcal{P}_{\mathbf{O}(n)}[(\mathbf{A}_k\mathbf{Y})^{\circ 3}\mathbf{Y}^*]. \quad (18)$$

**The sequence  $\mathbf{A}_k$  converges locally to  $\mathbf{A}_\star$  with a cubic rate.**

# Minimizing a Concave Function on a Stiefel Manifold

Consider a concave function  $f(\mathbf{X})$  over the Stiefel Manifold:

$$\mathbf{V}_m(\mathbb{R}^n) \doteq \{\mathbf{X} \in \mathbb{R}^{n \times m} \mid \mathbf{X}^* \mathbf{X} = \mathbf{I}_{m \times m}\}.$$

Then for the program:

$$\min_{\mathbf{X}} f(\mathbf{X}) \quad \text{subject to} \quad \mathbf{X}^* \mathbf{X} = \mathbf{I}, \quad (19)$$

we consider the Lagrangian:

$$\mathcal{L}(\mathbf{X}, \mathbf{\Lambda}) \doteq f(\mathbf{X}) + \langle \mathbf{\Lambda}, \mathbf{X}^* \mathbf{X} - \mathbf{I} \rangle. \quad (20)$$

The necessary condition for optimality  $\nabla_{\mathbf{X}} \mathcal{L}(\mathbf{X}, \mathbf{\Lambda}) = \mathbf{0}$  gives

$$-\nabla f(\mathbf{X}) = \mathbf{X} \mathbf{S}, \quad (21)$$

for a symmetric matrix  $\mathbf{S} = (\mathbf{\Lambda} + \mathbf{\Lambda}^*)$ .

## Generalized Power Iteration

Since  $\mathbf{X}^* \mathbf{X} = \mathbf{I}$ , this gives  $\nabla f(\mathbf{X})^* \nabla f(\mathbf{X}) = \mathbf{S}^* \mathbf{X}^* \mathbf{X} \mathbf{S} = \mathbf{S}^2$  hence  $\mathbf{S} = [\nabla f(\mathbf{X})^* \nabla f(\mathbf{X})]^{1/2}$ . When  $\mathbf{S}$  is invertible, the necessary condition (21) for optimality becomes:

$$\mathbf{X} = -\nabla f(\mathbf{X})[\nabla f(\mathbf{X})^* \nabla f(\mathbf{X})]^{-1/2}. \quad (22)$$

This gives a mapping from  $\mathbf{V}_m(\mathbb{R}^n)$  to itself:

$$g(\mathbf{X}) \doteq -\nabla f(\mathbf{X})[\nabla f(\mathbf{X})^* \nabla f(\mathbf{X})]^{-1/2} : \mathbf{V}_m(\mathbb{R}^n) \rightarrow \mathbf{V}_m(\mathbb{R}^n). \quad (23)$$

The optimal fixed point solution can be computed with the iteration:

$$\mathbf{X}_{k+1} = g(\mathbf{X}_k) = -\nabla f(\mathbf{X}_k)[\nabla f(\mathbf{X}_k)^* \nabla f(\mathbf{X}_k)]^{-1/2}. \quad (24)$$

**$\mathbf{X}_k$  converges to a critical point with a rate  $O(1/k)$ .**<sup>2</sup>

---

<sup>2</sup>Generalized power method for sparse principal component analysis, M. Journée, Y. Nesterov, P. Richtarik, and R. Sepulchre, *Journal of Machine Learning Research*, 2010.



# Fixed Point of a Contracting Mapping

let  $\mathcal{M}$  be a compact smooth manifold with a distance metric  $d(\cdot, \cdot)$ .

## Definition (Contraction Mapping)

A map  $g : \mathcal{M} \rightarrow \mathcal{M}$  is called a contraction mapping on  $\mathcal{M}$  if there exists  $\rho \in (0, 1)$  such that  $d(g(\mathbf{x}), g(\mathbf{y})) \leq \rho \cdot d(\mathbf{x}, \mathbf{y})$  for all  $\mathbf{x}, \mathbf{y} \in \mathcal{M}$ .

## Theorem (Banach-Caccioppoli Fixed Point)

*Let  $(\mathcal{M}, d)$  be a complete metric space with a contraction mapping:  $g : \mathcal{M} \rightarrow \mathcal{M}$ . Then  $g$  has a unique fixed point  $\mathbf{x}_\star \in \mathcal{M}$ :  $g(\mathbf{x}_\star) = \mathbf{x}_\star$ .*

The unique fixed point  $\mathbf{x}_\star$  can be found through iteration:

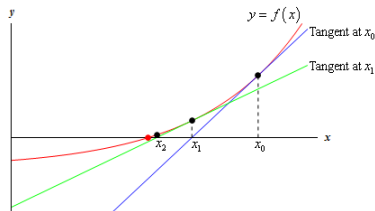
$$\mathbf{x}_{k+1} \leftarrow g(\mathbf{x}_k), \quad k = 0, 1, \dots$$

with  $\mathbf{x}_k \rightarrow \mathbf{x}_\star$  at least geometrically.

# Back to the Origin

Newton's Method: finding the zero  $x_*$  of a function  $f(x)$  such that  $f(x_*) = 0$  as a fixed point to the mapping:

$$g(x) \doteq x - \frac{f(x)}{f'(x)}. \quad (25)$$



The Newton iteration is just:

$$x_{k+1} = g(x_k) = x_k - \frac{f(x_k)}{f'(x_k)}. \quad (26)$$

**Applying to  $\min f(x)$  or equivalently solving  $f'(x) = 0$  leads to Newton descent!**

# Assignments

- Reading: Section 9.6 of Chapter 9.
- Written Homework #4.