

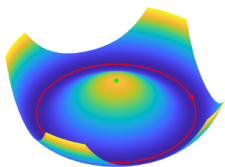
Computational Principles for High-dim Data Analysis

(Lecture Eighteen)

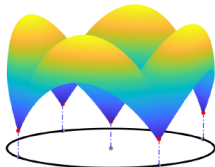
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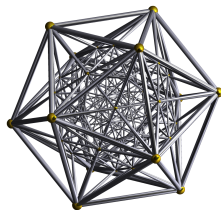
November 2, 2021



Rotational symmetry



Discrete symmetry



Nonconvex Optimization for High-Dim Problems

Fixed Point Power Iteration

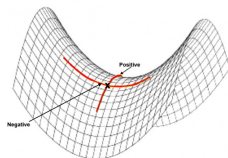
1 Power Iteration is Everywhere

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

Negative Curvature and Newton Descent

Consider a nonconvex program:

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



Negative curvature descent: compute e_k satisfying $\mathbf{A}e_k = \lambda_{\max}(\mathbf{A})e_k$ 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:

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

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

Power iteration:

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

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

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

Two gradient evaluations per power iteration.

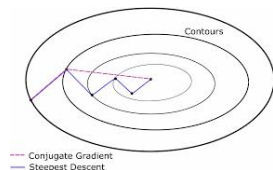
Conjugate Gradient Descent

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:¹ 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 $i = 0, 1, 2, \dots$:

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



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

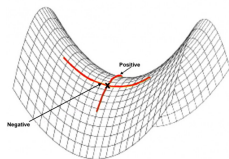
Effect of Noisy Gradient around a Saddle Point

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:

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

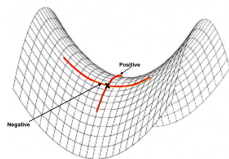
Since $\lambda_{\max}(\mathbf{A}) = 1 - \lambda_{\min}(\mathbf{H})/L_1 > 1$, this is **an unstable linear dynamic system** with random noise as the input:

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

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:

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

- Algorithm:

$$\mathbf{w}_{t+1} = \mathcal{P}_{\mathbb{S}^{n-1}} [\nabla_{\mathbf{w}} \varphi(\mathbf{w}_t)] = \frac{\mathbf{Y} \mathbf{Y}^* \mathbf{w}_t}{\|\mathbf{Y} \mathbf{Y}^* \mathbf{w}_t\|_2}$$

- **ICA**

- Optimization:

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

- Algorithm:

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

- **DL**

- Optimization:

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

- Algorithm:

$$\mathbf{W}_{t+1} = \mathcal{P}_{\text{St}(k, n; \mathbb{R})} [\nabla_{\mathbf{W}} \phi(\mathbf{W}_t)] = \mathbf{U}_t \mathbf{V}_t^*,$$

where $\mathbf{U}_t \boldsymbol{\Sigma}_t \mathbf{V}_t^* = \text{SVD}[\mathbf{Y} (\mathbf{Y}^* \mathbf{W})^{\circ 3}]$.

Singular Vectors via Nonconvex Optimization

To compute singular vector, say \mathbf{u}_1 , consider the optimization problem:

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

with $\mathbf{\Gamma} \doteq \mathbf{Y}\mathbf{Y}^*$.

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 φ 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 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 λ_2/λ_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 $O(1/k)$.²

²Generalized 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:

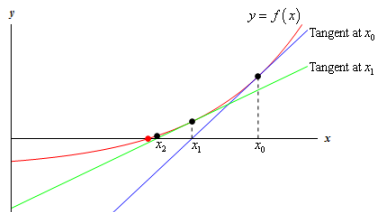
$$\mathbf{x}_{k+1} \leftarrow g(\mathbf{x}_k), \quad k = 0, 1, \dots$$

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.