

Gradient algorithms

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Why should I bother to learn this stuff?

- Gradient algorithm is the easiest, most robust optimization algorithm. It is not numerically efficient, but numerous more advanced algorithms are built on it.
- Conjugate gradient algorithm(s) are efficient methods for (quasi)-quadratic function. They are in particular used for approximately solving large linear systems.
- \implies useful for comprehension of
 - ▶ more advanced continuous optimization algorithms
 - ▶ machine learning training methods
 - ▶ numerical methods for solving discretized PDE

Contents

- 1 Descent methods and black-box optimization [BV 9.1]
 - Some general thoughts and definition
 - Descent methods
- 2 Strong convexity consequences [BV 9.2]
- 3 Gradient descent [BV 9.3-9.4]
- 4 Conjugate gradient [JCG - 8.2]

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A word on solution

- In this lecture, we are going to address **unconstrained**, finite dimensional, non-linear, smooth, optimization problem.
- In continuous non-linear (and non-quadratic) optimization, we cannot expect to obtain an *exact* solution. We are thus looking for approximate solutions.
- By solution, we generally mean local minimum.¹
- The speed of convergence of an algorithm is thus determining an upper bound on the number of iterations required to get an ε -solution, for $\varepsilon > 0$.

¹Sometimes just stationary points. Equivalent to global minimum in the convex setting.

Black-box optimization



We consider the following unconstrained optimization problem

$$\underset{x \in \mathbb{R}^n}{\text{Min}} \quad f(x)$$

- The **black-box** model consists in considering that we only know the function f through an **oracle**, that is a way of computing information on f at a given point x .
- Oracle gives local information on f . Oracles are generally given as user-defined code.
 - ▶ A *zeroth* order oracle only return the value $f(x)$.
 - ▶ A *first* order oracle return both $f(x)$ and $\nabla f(x)$.
 - ▶ A *second* order oracle return $f(x)$, $\nabla f(x)$ and $\nabla^2 f(x)$.
- By opposition, **structured optimization** leverage more knowledge on the objective function f . Classical models are
 - ▶ $f(x) = \sum_{i=1}^N f_i(x)$;
 - ▶ $f(x) = f_0(x) + \lambda g(x)$, where $f_0(x)$ is smooth and g is "simple", typically $g(x) = \|x\|_1$;
 - ▶ ...

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Descent methods

Consider the unconstrained optimization problem

$$v^\sharp = \min_{x \in \mathbb{R}^n} f(x).$$

A *descent direction algorithm* is an algorithm that constructs a sequence of points $(x^{(k)})_{k \in \mathbb{N}}$, that are recursively defined with:

$$x^{(k+1)} = x^{(k)} + t^{(k)} d^{(k)}$$

where

- $x^{(0)}$ is the initial point,
- $d^{(k)} \in \mathbb{R}^n$ is the descent direction,
- $t^{(k)}$ is the step length.

For most of the analysis, we will assume f to be (strongly) convex, but the algorithms presented are often used in a non-convex setting.

To complete the algorithm, we need a **stopping test**, generally testing that $\|\nabla f(x^{(k)})\|$ is small enough.

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To complete the algorithm, we need a **stopping test**, generally testing that $\|\nabla f(x^{(k)})\|$ is small enough.



For a differentiable objective function f , $d^{(k)}$ will be a descent direction iff $\nabla f(x^{(k)}) \cdot d^{(k)} < 0$, which can be seen from a first order development:

$$f(x^{(k)} + t^{(k)} d^{(k)}) = f(x^{(k)}) + t \langle \nabla f(x^{(k)}), d^{(k)} \rangle + o(t).$$

The most classical descent direction are²

- ① $d^{(k)} = -\nabla f(x^{(k)})$ (gradient)
- ② $d^{(k)} = -\nabla f(x^{(k)}) + \beta^{(k)} d^{(k-1)}$ (conjugate gradient)
- ③ $d^{(k)} = -\alpha^{(k)} \nabla f(x^{(k)}) + \beta^{(k)} (x^{(k)} - x^{(k-1)})$ (heavy ball \diamond)
- ④ $d^{(k)} = -[\nabla^2 f(x^{(k)})]^{-1} \nabla f(x^{(k)})$ (Newton)
- ⑤ $d^{(k)} = -W^{(k)} \nabla f(x^{(k)})$ (Quasi-Newton)
where $W^{(k)} \approx [\nabla^2 f(x^{(k)})]^{-1}$.

²they will be discussed at length during the course



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The step-size $t^{(k)}$ can be:

- **fixed** $t^{(k)} = t^{(0)}$,
 - ▶ too small and it will take forever
 - ▶ too large and it won't converge
- **optimal** $t^{(k)} \in \arg \min_{\tau \geq 0} f(x^{(k)} + \tau d^{(k)})$,
 - ▶ computing it requires solving a unidimensional problem
 - ▶ might not be worth the computation
- a **backtracking or receding step** choice³, for given $\tau_0 > 0, \alpha \in]0, 0.5[, \beta \in]0, 1[$,
 - 1 $\tau = \tau_0$
 - 2 if $f(x^{(k)} + \tau d^{(k)}) < f(x^{(k)}) + \alpha \tau \nabla f(x^{(k)})^\top d^{(k)}$: $t^{(k)} = \tau$, STOP
 - 3 $\tau \leftarrow \beta \tau$, go back to 2.
 - ▶ start with an "optimist" step τ_0
 - ▶ automatically adapts to ensure convergence
 - ▶ more complex procedure exists

³There exists a lot of other alternatives

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Strong convexity definition(s)



Recall that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is m -convex⁴ iff

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y) - \frac{m}{2}t(1-t)\|y-x\|^2, \quad \forall x, y, \quad \forall t \in]0, 1[$$

If f is differentiable, it is m -convex iff

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{m}{2}\|y - x\|^2, \quad \forall y, x$$

If f is twice differentiable, it is m -convex iff

$$mI \preceq \nabla^2 f(x) \quad \forall x$$

iff

$$m \leq \lambda \quad \forall \lambda \in \text{sp}(\nabla^2 f(x)), \quad \forall x$$

→ this last characterization is the most useful for our analysis.

⁴A strongly convex function is a m -convex function for some $m > 0$

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Bounding the Hessian

Consider a m -convex \mathcal{C}^2 function (on its domain), and $x^{(0)} \in \text{dom } f$. Denote $S := \text{lev}_{f(x_0)}(f) = \{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\}$.

As f is a strongly convex function S is bounded.

As $\nabla^2 f$ is continuous, there exists $M > 0$ such that, $\|\nabla^2 f(x)\| \leq M$, for all $x \in S$.

Thus we have, for all $x \in S$,

$$mI \preceq \nabla^2 f(x) \preceq MI$$

Or equivalently

$$m \leq \lambda_{\min}(\nabla^2 f(x)) \leq \lambda_{\max}(\nabla^2 f(x)) \leq M \quad \forall x \in S$$

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Strongly convex suboptimality certificate



Let f be a m -convex \mathcal{C}^2 function. We have

$$f(y) \geq f(x) + \langle \nabla f(x), y - x \rangle + \frac{m}{2} \|y - x\|^2, \quad \forall y, x$$

The under approximation is minimized, for a given x , for $y^\# = x - \frac{1}{m} \nabla f(x)$, yielding

$$f(y) \geq f(x) - \frac{1}{2m} \|\nabla f(x)\|^2 \quad \forall y$$

$$v^\# + \frac{1}{2m} \|\nabla f(x)\|^2 \geq f(x) \quad \forall x$$

Thus we obtain the following sub-optimality certificate

$$\|\nabla f(x)\| \leq \sqrt{2m\varepsilon} \implies f(x) \leq v^\# + \varepsilon$$

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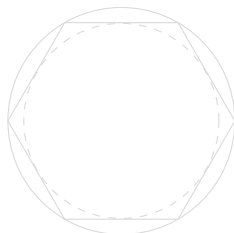


For any $A \in S_n^{++}$ positive definite matrix, we define its **condition number** $\kappa(A) = \lambda_{\max}/\lambda_{\min} \geq 1$ the ratio between its largest and smallest eigenvalue.

Consider a bounded convex set C . Let D_{out} be the diameter of the smallest ball B_{out} containing C , and D_{in} be the diameter of the largest ball B_{in} contained in C .

Then the **condition number** of C is

$$\text{cond}(C) = \left(\frac{D_{out}}{D_{in}} \right)^2$$



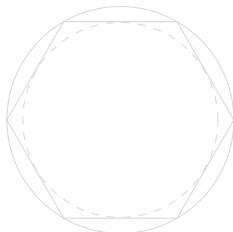


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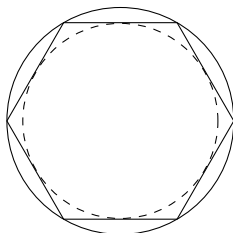


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Condition number of sublevel set



We have, for all $x \in S$,

$$mI \preceq \nabla^2 f(x) \preceq MI$$

thus

$$\kappa(\nabla^2 f(x)) \leq M/m$$

Further,

$$v^\# + \frac{m}{2} \|x - x^\#\|^2 \leq f(x) \leq v^\# + \frac{M}{2} \|x - x^\#\|^2$$

For any $v^\# \leq \alpha \leq f(x_0)$, we have

$$B\left(x^\#, \sqrt{2(\alpha - v^\#)/M}\right) \subset \underset{\alpha}{\text{lev}} f \subset B\left(x^\#, \sqrt{2(\alpha - v^\#)/m}\right)$$

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- The gradient descent algorithm is a first-order descent direction algorithm with $d^{(k)} = -\nabla f(x^{(k)})$.
- That is, with an initial point x_0 , we have

$$x^{(k+1)} = x^{(k)} - t^{(k)} \nabla f(x^{(k)}).$$

- The three step-size choices (fixed, optimal and decreasing) lead to variations of the algorithm.
- This algorithm is **slow**, but robust in the sense that it often ends up converging.
- Most implementations of advanced algorithms have fail-safe procedures that default to a gradient step when something goes wrong for numerical reasons.
- It is the basis of the stochastic-gradient algorithm, which is used (in advanced form) to train ML models.



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- Using the linear approximation

$f(\mathbf{x}^{(k)} + \mathbf{h}) = f(\mathbf{x}^{(k)}) + \nabla f(\mathbf{x}^{(k)})^\top \mathbf{h} + o(\|\mathbf{h}\|_{\mathfrak{X}})$, it is quite natural to look for the **steepest descent** direction, that is

$$\mathbf{d}^{(k)} \in \arg \min_{\mathbf{h}} \left\{ \nabla f(\mathbf{x}^{(k)})^\top \mathbf{h} \mid \|\mathbf{h}\|_{\mathfrak{X}} \leq 1 \right\}$$

- Here $\|\cdot\|_{\mathfrak{X}}$ could be any norm on \mathbb{R}^n .

- ▶ If $\|\cdot\|_{\mathfrak{X}} = \|\cdot\|_2$, the steepest descent is a gradient step, i.e. proportional to $-\nabla f(\mathbf{x}^{(k)})$.
- ▶ If $\|\cdot\|_{\mathfrak{X}} = \|\cdot\|_P$, $\|\mathbf{x}\|_{\mathfrak{X}} = \|P^{1/2}\mathbf{x}\|_2$ for some $P \in S_{++}^n$, then the steepest descent is $-P^{-1}\nabla f(\mathbf{x}^{(k)})$. In other words, a steepest descent step is a gradient step done on a problem after a change of variable $\bar{\mathbf{x}} = P^{1/2}\mathbf{x}$.
- ▶ If $\|\cdot\|_{\mathfrak{X}} = \|\cdot\|_1$, then the steepest descent can be chosen along a single coordinate, leading to the **coordinate descent algorithm**.

♠ Exercise: Prove these results.



Assume that f is such that $0 \preceq \nabla^2 f \preceq MI$.

Theorem

The gradient algorithm with fixed step size $t^{(k)} = t \leq \frac{1}{M}$ satisfies

$$f(x^{(k)}) - v^\# \leq \frac{2M\|x^{(0)} - x^\#\|}{k} = O(1/k)$$

\leadsto this is a *sublinear* rate of convergence.

Convergence results - strongly convex case



Assume that f is such that $mI \preceq \nabla^2 f \preceq MI$, with $m > 0$. Define the conditioning factor $\kappa = M/m$.

Theorem

If $x^{(k)}$ is obtained from the optimal step, we have

$$f(x^{(k)}) - v^\# \leq C^k (f(x_0) - v^\#), \quad C = 1 - 1/\kappa$$

If $x^{(k)}$ is obtained by receding step size we have

$$f(x^{(k)}) - v^\# \leq C^k (f(x_0) - v^\#), \quad C = 1 - \min \{2m\alpha, 2\beta\alpha\} / \kappa$$

\leadsto linear rate of convergence.

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The gradient conjugate algorithm stems from looking for numerical solutions to the linear equation

$$Ax = b$$

- Never, ever, compute A^{-1} to solve a linear system.
- Classical algebraic methods do a methodological factorization of A to obtain the (exact) value of x .
- These methods are in $O(n^3)$ operations. They only yield a solution at the end of the algorithm.
- The solution would be exact if there were no rounding errors...

Alternatively, we can look to solve

$$\underset{x \in \mathbb{R}^n}{\text{Min}} \quad f(x) := \frac{1}{2} x^\top A x - b^\top x$$

which is a smooth, unconstrained, convex optimization problem, whose optimal solution is given by $Ax = b$.

We will assume that $A \in S_{++}^n$. If A is non symmetric, but invertible, we could consider $A^\top Ax = A^\top b$.

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Conjugate directions



We say that $u, v \in \mathbb{R}^n$ are **A-conjugate** if they are orthogonal for the scalar product associated to A , i.e.

$$\langle u, v \rangle_A := u^\top A v = 0$$

Let $(\tilde{d}_i)_{i \in [k]}$ be a linearly independent family of vector. We can construct a family of conjugate directions $(d_i)_{i \in [k]}$ through the Gram-Schmidt procedure (without normalization), i.e., $\tilde{d}_1 = d_1$, and

$$d_\kappa = \tilde{d}_\kappa - \sum_{i=1}^{\kappa-1} \beta_{i,\kappa} d_i$$

where

$$\beta_{i,\kappa} = \frac{\langle \tilde{d}_\kappa, d_i \rangle_A}{\langle d_i, d_i \rangle_A} = \frac{\tilde{d}_\kappa^\top A d_i}{d_i^\top A d_i}$$

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We say that $u, v \in \mathbb{R}^n$ are A -conjugate if they are orthogonal for the scalar product associated to A , i.e.

$$\langle u, v \rangle_A := u^\top A v = 0$$

Let $(\tilde{d}_i)_{i \in [k]}$ be a linearly independent family of vector. We can construct a family of conjugate directions $(d_i)_{i \in [k]}$ through the Gram-Schmidt procedure (without normalization), i.e., $\tilde{d}_1 = d_1$, and

$$d_\kappa = \tilde{d}_\kappa - \sum_{i=1}^{\kappa-1} \beta_{i,\kappa} d_i$$

where

$$\beta_{i,\kappa} = \frac{\langle \tilde{d}_\kappa, d_i \rangle_A}{\langle d_i, d_i \rangle_A} = \frac{\tilde{d}_\kappa^\top A d_i}{d_i^\top A d_i}$$

Conjugate direction method for quadratic function



Consider, for $A \in S_{++}^n$

$$f(x) := \frac{1}{2} x^\top A x - b^\top x$$

A conjugate direction algorithm is a descent direction algorithm such that,

$$x^{(k+1)} = \arg \min_{x \in x_1 + E^{(k)}} f(x)$$

where

$$E^{(k)} = \text{vect}(d^{(1)}, \dots, d^{(k)})$$

♠ Exercise: Denote $g^{(k)} = \nabla f(x^{(k)})$. Show that

- ① $g^{(k)\top} d_i = 0$ for $i < k$
- ② $g^{(k+1)} = g^{(k)} + t^{(k)} A d^{(k)}$
- ③ $g^{(k)\top} d^{(i)} + t^{(k)} d^{(k)\top} A d^{(i)} = 0$ for $i \leq k$
- ④ Either
 - ▶ $g^{(k)\top} d^{(k)} = 0$ and $t^{(k)} = 0$
 - ▶ or $g^{(k)\top} d^{(k)} < 0$ and $t^{(k)} = -\frac{g^{(k)\top} d^{(k)}}{d^{(k)\top} A d^{(k)}}$

Data: Linearly independent direction $\tilde{d}^{(1)}, \dots, \tilde{d}^{(n)}$, initial point $x^{(1)}$

Matrix A and vector b

for $k \in [n]$ **do**

$$d^{(k)} = \tilde{d}^{(k)} - \sum_{i=1}^{k-1} \frac{\langle \tilde{d}^{(k)}, d^{(i)} \rangle_A}{\langle d^{(i)}, d^{(i)} \rangle_A} d^{(i)} ; \quad // \text{ A-orthogonalisation}$$

$$t^{(k)} = \frac{\nabla f(x^{(k)})^\top d^{(k)}}{\langle d^{(k)}, d^{(k)} \rangle_A} ; \quad // \text{ optimal step}$$

$$x^{(k+1)} = x^{(k)} + t^{(k)} d^{(k)}$$

Algorithm 1: Conjugate direction algorithm

This algorithm is such that (for a quadratic function f)

$$x^{(k+1)} = \arg \min_{x \in x_1 + E^{(k)}} f(x)$$

where

$$E^{(k)} = \text{vect}(d^{(1)}, \dots, d^{(k)})$$

Conjugate gradient algorithm - quadratic function



The conjugate gradient algorithm set $\tilde{d}^{(k)} = - \underbrace{\nabla f(x^{(k)})}_{:=g^{(k)}}$.

In particular, we obtain that $E^{(k)} = \text{vect}(g^{(1)}, \dots, g^{(k)})$, and thus

$$g^{(k)\top} g^{(i)} = 0 \quad \forall i \neq k$$

Note that

$$g^{(i+1)} - g^{(i)} = t^{(i)} A d^{(i)}, \quad \text{thus} \quad \frac{\langle \tilde{d}^{(k)}, d^{(i)} \rangle_A}{\langle d^{(i)}, d^{(i)} \rangle_A} = \frac{(\tilde{d}^{(k)})^\top (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})}$$

Thus, through orthogonality we have

$$\begin{aligned} d^{(k)} &= \tilde{d}^{(k)} - \sum_{i=1}^{k-1} \frac{-g^{(k)\top} (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})} d^{(i)} \\ &= -g^{(k)} + \frac{g^{(k)\top} (g^{(k)} - g^{(k-1)})}{d^{(k-1)\top} (g^{(k)} - g^{(k-1)})} d^{(k-1)} = -g^{(k)} + \frac{\|g^{(k)}\|^2}{\|g^{(k-1)}\|^2} d^{(k-1)} \end{aligned}$$

Conjugate gradient algorithm - quadratic function



The conjugate gradient algorithm set $\tilde{d}^{(k)} = \underbrace{-\nabla f(x^{(k)})}_{:=g^{(k)}}$.

In particular, we obtain that $E^{(k)} = \text{vect}(g^{(1)}, \dots, g^{(k)})$, and thus

$$g^{(k)\top} g^{(i)} = 0 \quad \forall i \neq k$$

Note that

$$g^{(i+1)} - g^{(i)} = t^{(i)} A d^{(i)}, \quad \text{thus} \quad \frac{\langle \tilde{d}^{(k)}, d^{(i)} \rangle_A}{\langle d^{(i)}, d^{(i)} \rangle_A} = \frac{(\tilde{d}^{(k)})^\top (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})}$$

Thus, through orthogonality we have

$$\begin{aligned} d^{(k)} &= \tilde{d}^{(k)} - \sum_{i=1}^{k-1} \frac{-g^{(k)\top} (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})} d^{(i)} \\ &= -g^{(k)} + \frac{g^{(k)\top} (g^{(k)} - g^{(k-1)})}{d^{(k-1)\top} (g^{(k)} - g^{(k-1)})} d^{(k-1)} = -g^{(k)} + \frac{\|g^{(k)}\|^2}{\|g^{(k-1)}\|^2} d^{(k-1)} \end{aligned}$$

Conjugate gradient algorithm - quadratic function



The conjugate gradient algorithm set $\tilde{d}^{(k)} = \underbrace{-\nabla f(x^{(k)})}_{:=g^{(k)}}$.

In particular, we obtain that $E^{(k)} = \text{vect}(g^{(1)}, \dots, g^{(k)})$, and thus

$$g^{(k)\top} g^{(i)} = 0 \quad \forall i \neq k$$

Note that

$$g^{(i+1)} - g^{(i)} = t^{(i)} A d^{(i)}, \quad \text{thus} \quad \frac{\langle \tilde{d}^{(k)}, d^{(i)} \rangle_A}{\langle d^{(i)}, d^{(i)} \rangle_A} = \frac{(\tilde{d}^{(k)})^\top (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})}$$

Thus, through orthogonality we have

$$\begin{aligned} d^{(k)} &= \tilde{d}^{(k)} - \sum_{i=1}^{k-1} \frac{-g^{(k)\top} (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})} d^{(i)} \\ &= -g^{(k)} + \frac{g^{(k)\top} (g^{(k)} - g^{(k-1)})}{d^{(k-1)\top} (g^{(k)} - g^{(k-1)})} d^{(k-1)} = -g^{(k)} + \frac{\|g^{(k)}\|^2}{\|g^{(k-1)}\|^2} d^{(k-1)} \end{aligned}$$

Conjugate gradient algorithm - quadratic function



The conjugate gradient algorithm set $\tilde{d}^{(k)} = \underbrace{-\nabla f(x^{(k)})}_{:=g^{(k)}}$.

In particular, we obtain that $E^{(k)} = \text{vect}(g^{(1)}, \dots, g^{(k)})$, and thus

$$g^{(k)\top} g^{(i)} = 0 \quad \forall i \neq k$$

Note that

$$g^{(i+1)} - g^{(i)} = t^{(i)} A d^{(i)}, \quad \text{thus} \quad \frac{\langle \tilde{d}^{(k)}, d^{(i)} \rangle_A}{\langle d^{(i)}, d^{(i)} \rangle_A} = \frac{(\tilde{d}^{(k)})^\top (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})}$$

Thus, through orthogonality we have

$$\begin{aligned} d^{(k)} &= \tilde{d}^{(k)} - \sum_{i=1}^{k-1} \frac{-g^{(k)\top} (g^{(i+1)} - g^{(i)})}{d^{(i)\top} (g^{(i+1)} - g^{(i)})} d^{(i)} \\ &= -g^{(k)} + \frac{g^{(k)\top} (g^{(k)} - g^{(k-1)})}{d^{(k-1)\top} (g^{(k)} - g^{(k-1)})} d^{(k-1)} = -g^{(k)} + \frac{\|g^{(k)}\|^2}{\|g^{(k-1)}\|^2} d^{(k-1)} \end{aligned}$$

Data: Initial point $x^{(1)}$, matrix A and vector b

$$g^{(1)} = Ax^{(1)} - b ;$$

$d^{(1)} = -g^{(1)}$ **for** $k = 2..n$ **do**

 If $\|g^{(k)}\|_2^2$ is small : STOP;

$$d^{(k)} = -g^{(k)} + \frac{\|g^{(k)}\|_2^2}{\|g^{(k-1)}\|_2^2} d^{(k-1)} ;$$

$$t^{(k)} = \frac{\|g^{(k)}\|_2^2}{d^{(k)T} A d^{(k)}} ; \quad // \text{ optimal step}$$

$$x^{(k+1)} = x^{(k)} + t^{(k)} d^{(k)} ;$$

$$g^{(k+1)} = g^{(k)} + t^{(k)} A d^{(k)}$$

Algorithm 2: Conjugate gradient algorithm - quadratic function



We can show the following properties, for a quadratic function,

- The algorithm finds an optimal solution in at most n iterations
- If $\kappa = \lambda_{\max}/\lambda_{\min}$, we have

$$\|x^{(k+1)} - x^\# \|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \|x^{(1)} - x^\# \|_A$$

- By comparison, gradient descent with optimal step yields

$$\|x^{(k+1)} - x^\# \|_A \leq 2 \left(\frac{\kappa - 1}{\kappa + 1} \right)^k \|x^{(1)} - x^\# \|_A$$



Data: Initial point $x^{(1)}$, first order oracle

for $k \in [n]$ **do**

$$g^{(k)} = -\nabla f(x^{(k)}) ;$$

If $\|g^{(k)}\|_2^2$ is small : STOP;

$$d^{(k)} = -g^{(k)} + \beta^{(k)} d^{(k-1)} ;$$

$t^{(k)}$ obtained by receeding linear search ;

$$x^{(k+1)} = x^{(k)} + t^{(k)} d^{(k)} ;$$

Algorithm 3: Conjugate gradient algorithm - non-linear function

Two natural choices for the choice of β , equivalent for quadratic functions

$$\bullet \beta^{(k)} = \frac{\|g^{(k)}\|_2^2}{\|g^{(k-1)}\|_2^2} \quad (\text{Fletcher-Reeves})$$

$$\bullet \beta^{(k)} = \frac{g^{(k)\top} (g^{(k)} - g^{(k-1)})}{\|g^{(k-1)}\|_2^2} \quad (\text{Polak-Ribière})$$

What you have to know

- What is a descent direction method.
- That there is a step-size choice to make.
- That there exists multiple descent direction.
- Gradient method is the slowest method, and in most case you should used more advanced method through adapted library.
- Conditionning of the problem is important for convergence speed.

What you really should know

- A problem can be pre-conditioned through change of variable to get faster results.
- Solving linear system can be done exactly through algebraic method, or approximately (or exactly) through minimization method.
- Conjugate gradient method are efficient tools for (approximately) solving a linear equation.
- Conjugate gradient works by exactly minimizing the quadratic function on an affine subspace.

What you have to be able to do

- Implement a gradient method with receding step-size.

What you should be able to do

- Implement a conjugate gradient method.
- Use the strongly convex and/or Lipschitz gradient assumptions to derive bounds.