

Optimization in Machine Learning: Lecture 6

Solving Algorithm for Non-constrained Problems

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Gradient Descent Algorithm

Newton Method

4 Nesterov Acceleration



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1 Optimality Condition

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Starting from Least Squares



unconstrained minimization

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

- basic assumption
 - f is convex, twice continuously differentiable
 - the optimal value $p^* = \inf f(x)$ is attained
- example: Least Squares

$$\min_{x} \sum_{i=1}^{m} \left(a_i^{\mathsf{T}} x - y_i \right)^2$$

$$\min_{x} \|Ax - Y\|_{2}^{2} = \min_{x} (Ax - Y)^{\mathsf{T}} (Ax - Y)$$

Optimality Condition



unconstrained minimization

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

optimality condition

$$\nabla f(x) = 0$$

example: Least Squares

$$\nabla \|Ax - Y\|_2^2 = \nabla (Ax - Y)^{\mathsf{T}} (Ax - Y) = 2A^{\mathsf{T}} (Ax - Y) = 0$$



$$x^* = (A^\mathsf{T} A)^{-1} A^\mathsf{T} Y$$



Pseudo Inverse



unconstrained minimization

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

optimality condition

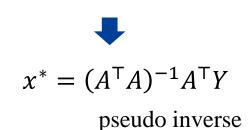
$$\nabla f(x) = 0$$

 $A(A^{T}A)^{-1}A^{T} = AA^{-1}(A^{T})^{-1}A^{T} = \mathbf{I}$ $(A^{T}A)^{-1}A^{T} = A^{-1}$

pseudo inverse = inverse?

example: Least Squares

$$\nabla \|Ax - Y\|_2^2 = \nabla (Ax - Y)^{\mathsf{T}} (Ax - Y) = 2A^{\mathsf{T}} (Ax - Y) = 0$$





Pseudo Inverse



unconstrained minimization

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

optimality condition

$$\nabla f(x) = 0$$

• example: Ridge Regression $\min_{x} ||Ax - Y||_{2}^{2} + \lambda ||x||_{2}^{2}$

$$\nabla \|Ax - Y\|_{2}^{2} + \lambda \|x\|_{2}^{2} = \nabla (Ax - Y)^{\mathsf{T}} (Ax - Y) + \lambda x^{\mathsf{T}} x = 2A^{\mathsf{T}} (Ax - Y) + 2\lambda x = 0$$



$$x^* = (\lambda \mathbf{I} + A^{\mathsf{T}} A)^{-1} A^{\mathsf{T}} Y$$

- ill-posed problem
- keep optimization property



Iterative Reweighted Least Squares

unconstrained minimization

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

optimality condition

analytical solution when the equation is linear

$$\nabla f(x) = 0$$
 · solving nonlinear equations > optimization

Iteratively Reweighted Least Squares

$$\min_{x} \sum_{i=1}^{m} p_i^k (a_i^{\mathsf{T}} x - y_i)^2 \longrightarrow x^{k+1} = (A^{\mathsf{T}} P^k A)^{-1} A^{\mathsf{T}} P^k Y$$

- approximate the function by a quadratic function
- link to Newton's method



Iterative Reweighted Least Squares

unconstrained minimization

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

optimality condition

analytical solution when the equation is linear

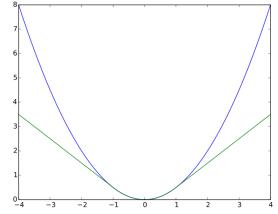
$$\nabla f(x) = 0$$
 · solving nonlinear equations > optimization

• Iteratively Reweighted Least Squares $L_{\text{huber}}(r) = \begin{cases} r^2/2 & \text{if } |r| < c \\ c(|r| - c/2) & \text{if } |r| \ge c \end{cases}$

example: Huber loss optimization

$$\min_{x} \quad \sum_{i=1}^{m} p_i^k (a_i^{\mathsf{T}} x - y_i)^2$$

- solution update $x^{k+1} = (A^T P^k A)^{-1} A^T P^k Y$
- weight update $p_i^{k+1} = \begin{cases} 1 & \text{if } |r_i| < c \\ c/r_i & \text{if } |r_i| \ge c \end{cases}$





Iterative Reweighted Least Squares

unconstrained minimization

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

optimality condition

$$\nabla f(x) = 0$$

Iteratively Reweighted Least Squares

the convergence should be carefully checked.

especially for non-smooth problem, e.g., in compressive sensing

$$\min_{x} \|Ax - Y\|_{2}^{2} + 2\lambda \|x\|_{1}$$

Ingrid Daubechies, et al. Iteratively reweighted least squares minimization for sparse recovery, *Communications on Pure and Applied Mathematics*, 2009

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Large Scale



- pseudo inverse $x^* = (A^T A)^{-1} A^T Y$
 - $A^{\mathsf{T}}A$ is an $n \times n$ matrix
 - inverse operation has complexity $O(n^3)$
- finding an analytical solution does not mean the problem is solved
- analytical solution could help if it could be efficiently calculated
- it is impossible for modern big data which may have million features

problem size	possible operations
small size	any operations
medium size	matrix inverse A^{-1}
large size	multiplication Ax
huge size	addition $x + y$



Yurii Nesterov



Descent Method



$\min f(x)$

• to produce a sequence of points $x^{(k)}$ to approach the optimum

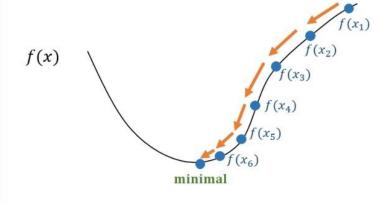
$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$
 with $f(x^{(k+1)}) < f(x^{(k)})$

General descent method.

given a starting point $x \in \operatorname{dom} f$. repeat

- 1. Determine a descent direction Δx .
- 2. Line search. Choose a step size t > 0.
- 3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.



https://zhuanlan.zhihu.com/p/36564434



Descent Method



min f(x)

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- 1. Determine a descent direction Δx .
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until stopping criterion is satisfied.

- staring point $x^{(0)}$
- descent direction $\Delta x^{(k)}$
- step size /step length/ learning rate $t^{(k)}$



Line Search



• when the direction $\Delta x^{(k)}$ is found, the update

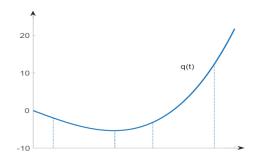
$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$

becomes a univariate problem to find the step length.

exact line search

$$t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$$

- the basic idea is to use bisection to compress the interval
- the key point is how to choose the breakpoint and how to judge the next interval

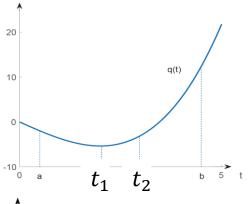


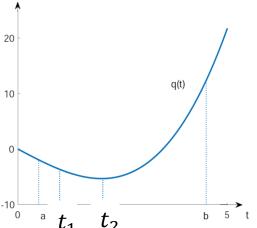


Line Search: by Function Value

$$t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$$

using at least two points, we can know where is the optimum





to have a constant compressive ratio *c*, the break point should satisfy

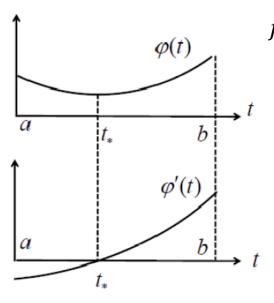
$$\frac{t_2 - a}{b - a} = \frac{b - t_1}{b - a} = c \qquad \frac{t_1 - a}{t_2 - a} = \frac{b - t_2}{b - t_1} = c$$

$$c = \frac{1}{2} \left(\sqrt{5} - 1 \right) \approx 0.618$$
golden-section

Line Search: by Gradient

$$t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$$

• if we know the gradient, we can improve the compressive ratio to c = 0.5



$$f'(t_*) = 0$$

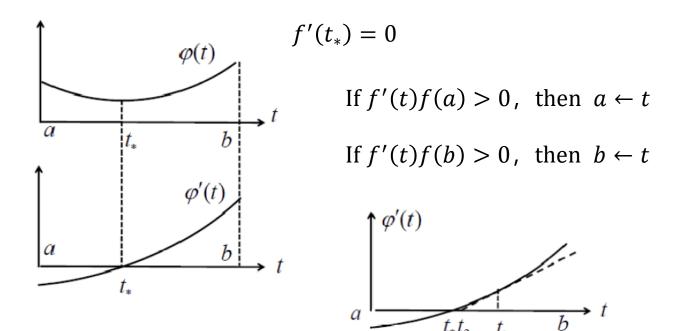
If
$$f'(t)f(a) > 0$$
, then $a \leftarrow t$

If
$$f'(t)f(b) > 0$$
, then $b \leftarrow t$

Line Search: by Gradient

$$t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$$

• if we know the gradient, we can improve the compressive ratio to c = 0.5



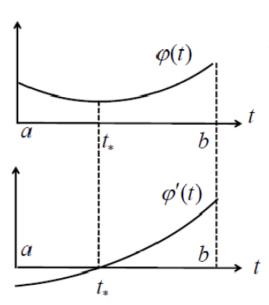
• if we know the second-order gradient, the convergence is very fast

Line Search: by Gradient



$$t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$$

• if we know the gradient, we can improve the compressive ratio to c = 0.5

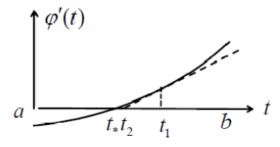


$$f'(t_*)=0$$

does that mean we should always use second-order gradient?

If
$$f'(t)f(a) > 0$$
, then $a \leftarrow t$

If
$$f'(t)f(b) > 0$$
, then $b \leftarrow t$



• if we know the second-order gradient, the convergence is very fast

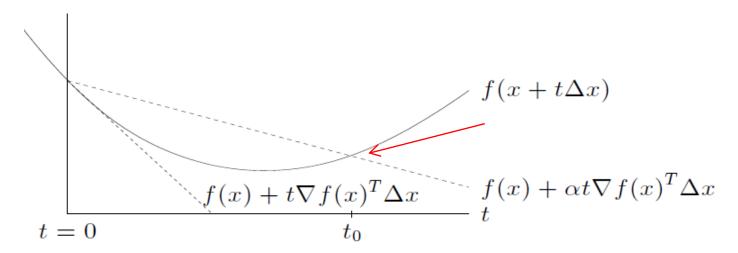
Line Search: Backtracking

- backtracking line search, with $\alpha \in (0,0.5), \beta \in (0,1)$
 - starting from t = 1, repeat $t = \beta t$, until

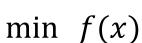
• exact search: $t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$



$$f(x + t\Delta x) < f(x) + \alpha t \nabla f(x)^{\mathsf{T}} \Delta x$$



Descent Direction



• to produce a sequence of points $x^{(k)}$ to approach the optimum

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$
 with $f(x^{(k+1)}) < f(x^{(k)})$

• if $\nabla f(x^{(k)})^{\mathsf{T}} \Delta x^{(k)} \ge 0$, from convexity

$$f\!\left(x^{(k+1)}\right) \geq f\!\left(x^{(k)}\right) + \nabla f \Delta x^{(k)} \geq 0$$

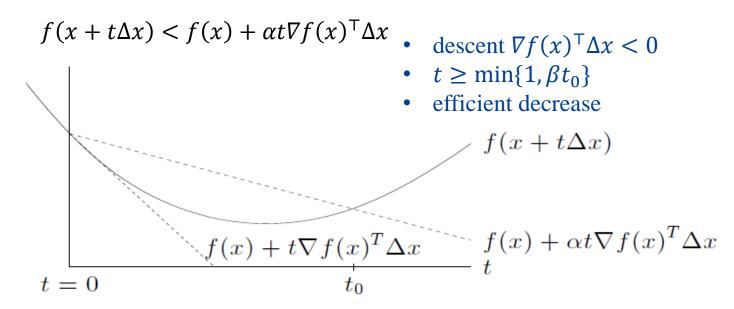


$$f(x^{(k+1)}) < f(x^{(k)}) \rightarrow \nabla f(x^{(k)})^{\mathsf{T}} \Delta x^{(k)} < 0$$



Line Search: Backtracking

- exact search: $t = \operatorname{argmin}_t f(x + t\Delta x) \triangleq q(t)$
- backtracking line search, with $\alpha \in (0,0.5), \beta \in (0,1)$
 - starting from t = 1, repeat $t = \beta t$, until



when t is small enough,

$$f(x + t\Delta x) \approx f(x) + t\nabla f(x)^{\mathsf{T}} \Delta x < f(x) + \alpha t \nabla f(x)^{\mathsf{T}} \Delta x$$



Descent Direction



• to produce a sequence of points $x^{(k)}$ to approach the optimum

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$
 with $f(x^{(k+1)}) < f(x^{(k)})$

• if $\nabla f(x^{(k)})^{\mathsf{T}} \Delta x^{(k)} \ge 0$, from convexity

$$f(x^{(k+1)}) \ge f(x^{(k)}) + \nabla f \Delta x^{(k)} \ge 0$$



$$f(x^{(k+1)}) < f(x^{(k)}) \rightarrow \nabla f(x^{(k)})^{\mathsf{T}} \Delta x^{(k)} < 0$$

• a natural choice is gradient: Gradient Descent algorithm

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



given a starting point $x \in \operatorname{dom} f$. repeat

- 1. $\Delta x := -\nabla f(x)$.
- 2. Line search. Choose step size t via exact or backtracking line search.
- 3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.

• stopping criterion: $\|\nabla f(x)\|_2 \le \varepsilon$



- convergence analysis
 - f is strongly convex on a set S: there exists an m > 0, such that

$$\nabla^2 f(x) \ge mI, \forall x \in S$$

• for any $x,y \in S$, there is

$$f(y) \ge f(x) + \nabla f(x)^{\mathsf{T}} (y - x) + \frac{m}{2} ||x - y||_2^2$$



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- stopping criterion: $\|\nabla f(x)\|_2 \le \varepsilon$
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• for any $x,y \in S$, there is

$$f(y) \ge f(x) + \nabla f(x)^{\mathsf{T}} (y - x) + \frac{m}{2} ||x - y||_2^2$$

how good the solution?bound the distance to the optimum

how fast the convergence?the convergence rate





solution quality

$$f(y) \ge f(x) + \nabla f(x)^{\mathsf{T}} (y - x) + \frac{m}{2} \|x - y\|_{2}^{2}$$

$$\ge f(x) + \nabla f(x)^{\mathsf{T}} (\tilde{y} - x) + \frac{m}{2} \|x - \tilde{y}\|_{2}^{2}$$

$$\ge f(x) - \frac{1}{2m} \|\nabla f(x)\|_{2}^{2}$$

TRH is a quadratic function on y,

take gradient, the minimum is at

$$\tilde{y} = x - \frac{1}{m} \nabla f(x)$$

• notice that the above holds for all y, then

$$f(x) - p^* \le \frac{1}{2m} \|\nabla f(x)\|_2^2$$

• the stopping criterion $\|\nabla f(x)\|_2 \le \varepsilon$ can control the distance to the optimum







from strong convexity and boundedness

$$mI \le \nabla^2 f(x) \le MI, \quad \forall x \in S$$

using the right equality, we have

$$f(x - t\nabla f(x)) \le f(x) - t\|\nabla f(x)\|_{2}^{2} + \frac{Mt^{2}}{2}\|\nabla f(x)\|_{2}^{2}$$

• with exact line search, we attain the best $t^* = \frac{1}{M}$, then

$$f(x - t\nabla f(x)) \le f(x) - \frac{1}{2M} \|\nabla f(x)\|_2^2$$

efficient decrease





efficient decrease

$$f(x^{(k+1)}) \le f(x^{(k)}) - \frac{1}{2M} \|\nabla f(x^{(k)})\|_{2}^{2}$$

solution quality

$$f(x^{(k)}) - p^* \le \frac{1}{2m} \|\nabla f(x^{(k)})\|_2^2$$

• therefore,

$$f(x^{(k+1)}) - p^* \le (1 - m/M)(f(x^{(k)}) - p^*)$$

iteratively update show that

$$f(x^{(k)}) - p^* \le (1 - c)^k (f(x^{(0)}) - p^*)$$
condition number initial guess
$$c = m/M$$

linear convergence(log err vs. iter curve is below a line)



the speed depends on the Hessian



from strong convexity and boundedness

$$mI \le \nabla^2 f(x) \le MI, \quad \forall x \in S$$

using the right equality, we have

$$f(x - t\nabla f(x)) \le f(x) - t\|\nabla f(x)\|_2^2 + \frac{Mt^2}{2}\|\nabla f(x)\|_2^2$$

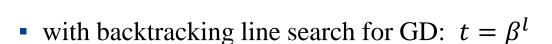
with backtracking line search for GD

$$f(x - t\nabla f(x)) < f(x) - \alpha t \|\nabla f(x)\|_2^2$$

when
$$0 \le t \le 1/M$$
, we have $-t + \frac{Mt^2}{2} \le -\frac{t}{2}$

$$f(x - t\nabla f(x)) \le f(x) - t\|\nabla f(x)\|_{2}^{2} + \frac{Mt^{2}}{2}\|\nabla f(x)\|_{2}^{2} \le f(x) - \frac{1}{2}t\|\nabla f(x)\|_{2}^{2}$$

since $\alpha \in (0,0.5)$, the backtracking condition can be satisfied by $0 \le t \le 1/M$



$$f(x - t\nabla f(x)) < f(x) - \alpha t \|\nabla f(x)\|_2^2$$

- if l = 0, then $f(x t\nabla f(x)) < f(x) \alpha ||\nabla f(x)||_2^2$
- if l > 1, then

$$f(x - \beta^{-1}t\nabla f(x)) > f(x) - \alpha\beta^{-1}t\|\nabla f(x)\|_{2}^{2}$$

$$f(x - \beta^{-1}t\nabla f(x)) \le f(x) - \beta^{-1}t\|\nabla f(x)\|_{2}^{2} + \frac{M(\beta^{-1}t)^{2}}{2}\|\nabla f(x)\|_{2}^{2}$$

we now have

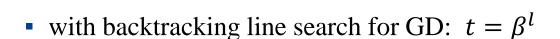
$$f(x - t\nabla f(x)) < f(x) - \min\{\alpha, \alpha\beta/M\} \|\nabla f(x)\|_2^2$$

$$-\alpha < -1 + \frac{M}{2}\beta^{-1}t$$

$$2(1-\alpha)\beta \quad \beta$$

$$t > \frac{2(1-\alpha)\beta}{M} > \frac{\beta}{M}$$





$$f(x - t\nabla f(x)) < f(x) - \alpha t \|\nabla f(x)\|_2^2$$

- if l = 0, then $f(x t\nabla f(x)) < f(x) \alpha ||\nabla f(x)||_2^2$
- if l > 1, then

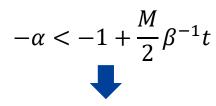
$$f(x - \beta^{-1}t\nabla f(x)) > f(x) - \alpha\beta^{-1}t\|\nabla f(x)\|_{2}^{2}$$

$$f(x - \beta^{-1}t\nabla f(x)) \le f(x) - \beta^{-1}t\|\nabla f(x)\|_{2}^{2} + \frac{M(\beta^{-1}t)^{2}}{2}\|\nabla f(x)\|_{2}^{2}$$

we now have

$$f(x - t\nabla f(x)) < f(x) - \min\{\alpha, \alpha\beta/M\} \|\nabla f(x)\|_2^2$$

$$f(x - t\nabla f(x)) \le f(x) - \frac{1}{2M} \|\nabla f(x)\|_2^2$$



$$t > \frac{2(1-\alpha)\beta}{M} > \frac{\beta}{M}$$

```
given a starting point x \in \operatorname{dom} f. repeat
```

- 1. $\Delta x := -\nabla f(x)$.
- 2. Line search. Choose step size t via exact or backtracking line search.
- 3. Update. $x := x + t\Delta x$.

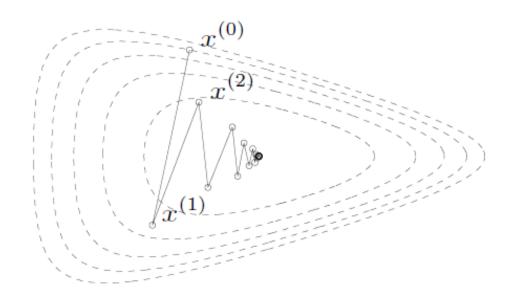
until stopping criterion is satisfied.

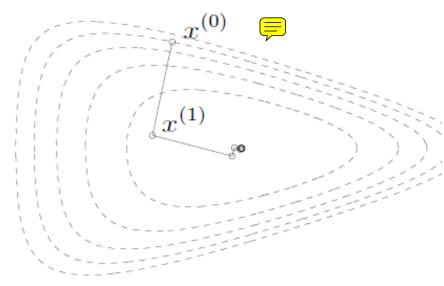
- line search (exact, backtracking)
- solution quality (strong convexity)
- linear convergence (strong convexity, boundedness)





$$f(x_1, x_2) = e^{x_1 + 3x_2 - 0.1} + e^{x_1 - 3x_2 - 0.1} + e^{-x_1 - 0.1}$$





backtracking line search

exact line search





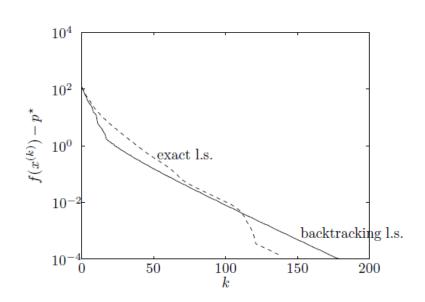
given a starting point $x \in \operatorname{dom} f$. repeat

- 1. $\Delta x := -\nabla f(x)$.
- 2. Line search. Choose step size t via exact or backtracking line search.
- 3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.

$$f(x) = c^T x - \sum_{i=1}^{500} \log(b_i - a_i^T x)$$

- line search (exact, backtracking)
- solution quality (strong convexity)
- linear convergence (strong convexity, boundedness)





```
given a starting point x \in \operatorname{dom} f. repeat
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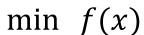
until stopping criterion is satisfied.

- line search (exact, backtracking)
- solution quality (strong convexity)
- linear convergence (strong convexity, boundedness)
- convergence speed relies on condition number $c = \frac{m}{M}$





Steepest Descent Method



• to produce a sequence of points $x^{(k)}$ to approach the optimum

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$
 with $f(x^{(k+1)}) < f(x^{(k)})$

$$f(x^{(k+1)}) \le f(x^{(k)}) + \nabla f(x^{(k)})^{\mathsf{T}} \Delta x^{(k)}$$

- which direction is the "best"
 - normalized steepest descent direction

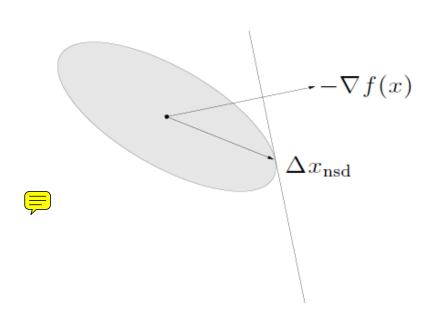
$$\Delta x_{\text{nsd}} = \operatorname{argmin}_{v} \{ \nabla f(x)^{\mathsf{T}} v, \text{s.t.} ||v|| = 1 \}$$

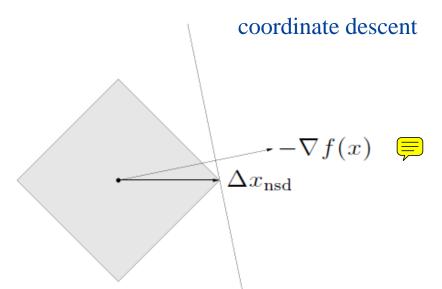
- projection of $-\nabla f(x)$ on the unit ball
- different norm corresponds to different directions



Steepest Descent Method







$$\Delta x_{\text{nsd}} = \operatorname{argmin}_{v} \{ \nabla f(x)^{\mathsf{T}} v, \text{s.t.} ||v|| = 1 \}$$



- projection of $-\nabla f(x)$ on the unit ball
- different norm corresponds to different directions



Sub-gradient for LASSO



$$\min_{x} \quad \gamma \sum_{j=1}^{n} |x_{j}| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_{i} - b_{i})^{2}$$

sub-gradient

$$\frac{\partial f}{\partial x} \in \lambda \frac{\partial \|x\|_1}{\partial x} + A^{\mathsf{T}} (Ax - Y)$$

optimality condition

$$0 \in \lambda \frac{\partial \|x\|_1}{\partial x} + A^{\mathsf{T}} (Ax - Y)$$

$$x = S_{\lambda}(x - A^{\mathsf{T}}(Ax - Y))$$

define shrinkage operator:

$$(S_{\lambda}(u))_{i} = \begin{cases} u_{i} - \lambda, & u(i) \ge \lambda \\ 0, & |u(i)| < \lambda \\ u_{i} + \lambda, & u(i) \le -\lambda \end{cases}$$



Iterative Soft Thresholding Algorithm

$$\min_{x} \quad \gamma \sum_{j=1}^{n} |x_{j}| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_{i} - b_{i})^{2}$$

optimality condition

$$x = S_{\lambda}(x - A^{\mathsf{T}}(Ax - Y))$$

iterative update

$$x^{k+1} = S_{\lambda} (x^k - A^{\mathsf{T}} (Ax^k - Y))$$

Convergence discussion for

$$x^{k+1} = T(x^k)$$

- a fixed point satisfies optimality condition
- the operator is non-expansive



Iterative Soft Thresholding Algorithm

$$x^{k+1} = S_{\lambda}(x^k - A^{\mathsf{T}}(Ax^k - Y))$$

a fixed point satisfies the optimality condition

$$x = S_{\lambda}(x - A^{\mathsf{T}}(Ax - Y))$$

non-expansive

$$T(x) \triangleq S_{\lambda}(x - A^{\mathsf{T}}(Ax - Y))$$

how to verify?

$$||S_{\lambda}(u) - S_{\lambda}(v)|| \le ||u - v||$$

$$||T(u) - T(v)|| = ||S_{\lambda}(u - A^{T}(Au - Y)) - S_{\lambda}(v - A^{T}(Av - Y))||$$

$$\leq ||u - A^{T}(Au - Y) - v + A^{T}(Av - Y)||$$

$$= ||(I - A^{T}A)u - (I - A^{T}A)v||$$

$$\leq ||I - A^{T}A|| ||u - v||$$
converge

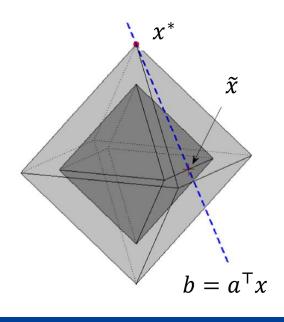
convergence condition: $||I - A^{T}A|| < 1$

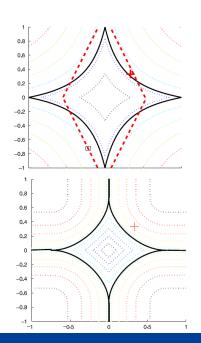


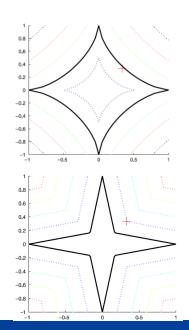
Off the convexity



- 11-norm is the best approximation among convex functions
- non-convex functions could enhance the sparsity









Off the convexity



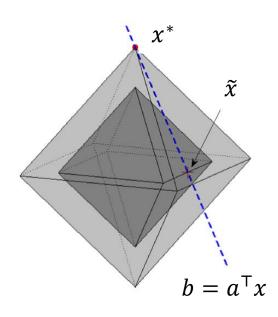
$$\min_{x} \quad \gamma \sum_{j=1}^{n} |x_{j}| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_{i} - b_{i})^{2}$$

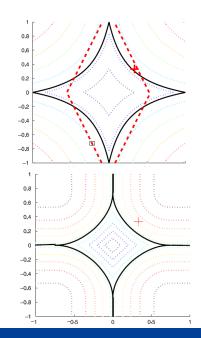
• in the view of iterative reweighted

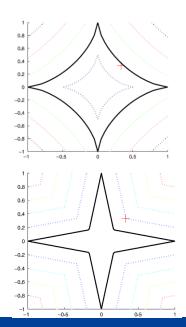
$$x^{k+1} = \underset{x}{\operatorname{argmin}} \quad \gamma \sum_{i=1}^{n} p_j^k |x_j| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_i - b_i)^2$$

How to design the weights?

 p_j^k is inverse proportional to $|x_j^k|$









Off the convexity



$$\min_{x} \quad \gamma \sum_{i=1}^{n} |x_{j}| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_{i} - b_{i})^{2}$$

• in the view of iterative reweighted

$$x^{k+1} = \underset{x}{\operatorname{argmin}} \quad \gamma \sum_{j=1}^{n} p_j^k |x_j| + \frac{1}{2} \sum_{i=1}^{m} (x^{\mathsf{T}} a_i - b_i)^2$$

 $||S_{\lambda,p}(u) - S_{\lambda,p}(v)|| ? ||u - v||$

• ISTA for non-convex penalty:

$$x^{k+1} = S_{\lambda,p^k} \left(x^k - A^{\mathsf{T}} (Ax^k - Y) \right)$$
$$\left(S_{\lambda,p}(u) \right)_i = \begin{cases} u_i - p_i \lambda, & u_i \ge p_i \lambda \\ 0, & |u(i)| < p_i \lambda \\ u_i + \lambda, & u(i) \le -p_i \lambda \end{cases}$$

$$u > v > 0$$

$$u - p_i(u)\lambda$$

$$v - p_i(v)\lambda$$

$$u - v >_{\text{possible}} u - p_i(u)\lambda$$

$$-(v - p_i(v)\lambda)$$

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GD: Staircase

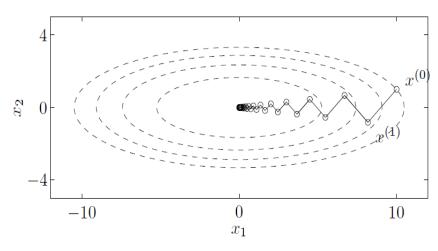


given a starting point $x \in \operatorname{dom} f$. repeat

- 1. $\Delta x := -\nabla f(x)$.
- 2. Line search. Choose step size t via exact or backtracking line search.
- 3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.

- gradient descent with exact line search results in "staircase"
 - the reason
 - when there is no
 - when it is worse





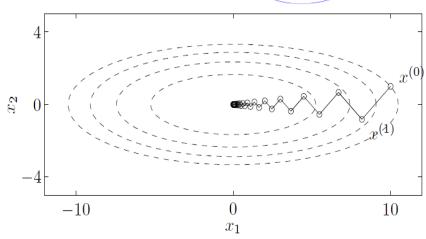
Adjustment



$$f(x^{(k)}) - p^* \le (1 - c)^k (f(x^{(0)}) - p^*)$$
condition number
$$c = m/M$$

- when there is no staircase: c = 1, i.e., the contour is a ball
- if not, we should adjust the descent direction, related to the condition number

$$\Delta x_{\rm nt} = -\nabla^2 f(x)^{-1} \nabla f(x)$$





Newton Step



$$\Delta x_{\rm nt} = -\nabla^2 f(x)^{-1} \nabla f(x)$$

how to prove?

- Newton step is a descent direction
- iteratively minimize the second approximation

$$f(x+v) \approx f(x) + \nabla f(x)^{\mathsf{T}} v + \frac{1}{2} v^{\mathsf{T}} \nabla^2 f(x) v$$



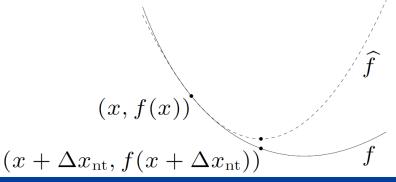


link to IRLS

$$\nabla f(x) + \nabla^2 f(x)v = 0$$



$$v^* = -\nabla^2 f(x)^{-1} \nabla f(x)$$





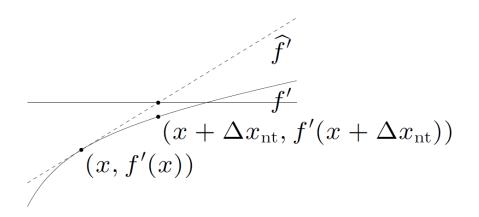
Newton Step

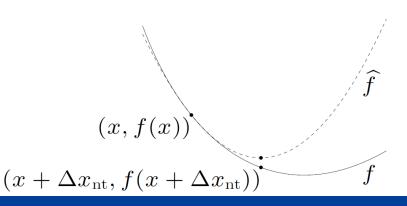


$$\Delta x_{\rm nt} = -\nabla^2 f(x)^{-1} \nabla f(x)$$

- Newton step is a descent direction
- iteratively solve the linearized optimality condition

$$\nabla f(x+v) \approx \nabla f(x)^{\mathsf{T}} + \nabla^2 f(x)v = 0$$







Newton Step



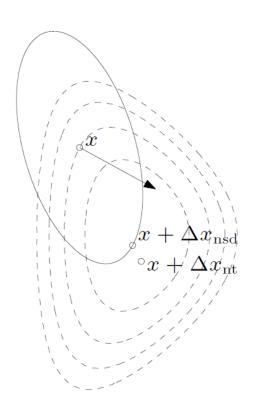
$$\Delta x_{\rm nt} = -\nabla^2 f(x)^{-1} \nabla f(x)$$

- Newton step is a descent direction
- steepest descent direction in local Hessian norm

$$\Delta x_{\mathrm{nt}} = \operatorname{argmin}_{v} \left\{ \nabla f(x)^{\mathsf{T}} v, \text{ s. t. } ||v||_{\nabla^{2} f(x)} = 1 \right\}$$

$$||v||_{\nabla^2 f(x)} = \sqrt{v^{\mathsf{T}} \nabla^2 f(x) v}$$

- modified Euclid distance



Newton Decrement



consider the quadratic approximation

$$f(x+v) \approx f(x) + \nabla f(x)^{\mathsf{T}} v + \frac{1}{2} v^{\mathsf{T}} \nabla^2 f(x) v \triangleq f(y)$$

the gap to the approximated optimum

$$f(x) - \inf_{y} f(y) = \frac{1}{2} \nabla f(x)^{\mathsf{T}} \nabla^{2} f(x)^{-1} \nabla f(x) \triangleq \frac{1}{2} \lambda(x)^{2}$$



Newton decrement

- Newton decrement is an estimation of $f(x) f^*$
- affine invariant: for $g(y) \triangleq f(Tx)$, they have the same Newton decrement

$$\lambda_g(y) = \lambda_f(x)$$

independent of linear changes of coordinates

(Damped) Newton's method



Gradient descent in Newton step with backtracking line search

given a starting point $x \in \operatorname{dom} f$, tolerance $\epsilon > 0$. repeat

- 1. Compute the Newton step and decrement.
 - $\Delta x_{\rm nt} := -\nabla^2 f(x)^{-1} \nabla f(x); \quad \lambda^2 := \nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x).$
- 2. Stopping criterion. quit if $\lambda^2/2 \leq \epsilon$.
- 3. Line search. Choose step size t by backtracking line search.
- 4. Update. $x := x + t\Delta x_{\rm nt}$.

- affine invariant: for $g(y) \triangleq f(Tx)$, they have the same Newton decrement
 - independent of linear changes of coordinates

$$y^0 = Tx^0 \qquad \Longrightarrow \qquad y^k = Tx^k$$

• how about the gradient descent?

Convergence analysis: Assumption

update

$$x^{k+1} = x^k + t^k d^k$$
 $d^k = \nabla^2 f(x^k)^{-1} \nabla f(x^k)$

strongly convexity and boundedness assumption

$$mI \le \nabla^2 f(x) \le MI, \quad \forall x \in S$$

Lipschitz continuous on the second order gradient

$$\|\nabla^2 f(y) - \nabla^2 f(x)\| \le L\|y - x\|, \forall x, y \in S$$

• to bound the gap between f(x) and its second-order approximation along d

$$f(x+d) = f(x) + \nabla f(x)^{\mathsf{T}} d + \frac{1}{2} d^{\mathsf{T}} \nabla^{2} f(x+\xi d) d, \quad \xi \in [0,1]$$

$$\left| f(x+d) - (f(x) + \nabla f(x)^{\mathsf{T}} d + \frac{1}{2} d^{\mathsf{T}} \nabla^{2} f(x) d) \right| = \left| d^{\mathsf{T}} \left(\nabla^{2} f(x+\xi d) - \nabla^{2} f(x) \right) d \right|$$

$$\leq \frac{1}{2} \left\| \nabla^{2} f(x+\xi d) - \nabla^{2} f(x) \right\| \|d\|^{2} \leq \frac{L}{2} \|\xi\| \|d\|^{3}$$

Convergence analysis: Assumption

update

$$x^{k+1} = x^k + t^k d^k$$
 $d^k = \nabla^2 f(x^k)^{-1} \nabla f(x^k)$

strongly convexity and boundedness assumption

$$mI \le \nabla^2 f(x) \le MI, \quad \forall x \in S$$

Lipschitz continuous on the second order gradient

$$\|\nabla^2 f(y) - \nabla^2 f(x)\| \le L\|y - x\|, \forall x, y \in S$$

• to bound the norm of the gradient

$$\frac{d\nabla f(x+td)}{dt} = \nabla^2 f(x+td)d$$

$$\int_0^1 (\nabla^2 f(x+td)d - \nabla^2 f(x)d) dt = \nabla f(x+td)$$

$$\nabla f(x) = \nabla^2 f(x)d$$

$$\|\nabla f(x+td)\| \le \int_0^1 Lt \|d\|^2 dt = \frac{L}{2} \|d\|^2 = \frac{L}{2} \|\nabla^2 f(x)^{-1} \nabla f(x)\|^2 \le \frac{L}{2m^2} \|\nabla f(x)\|^2$$

Convergence analysis: when backtracking stops

$$f(x + td) \le f(x) + \alpha \nabla f(x)^{\mathsf{T}} d$$

from Lipschitz condition

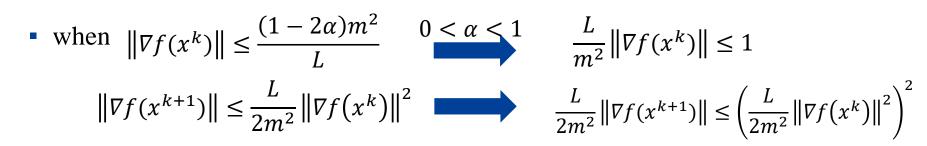
$$f(x) + \nabla f(x)^{\top} d - \frac{1}{2} \nabla f(x)^{\top} d + \frac{L}{2} ||d||^{3} \le f(x + td) \le f(x) + \alpha \nabla f(x)^{\top} d$$
$$\frac{1}{2} \nabla f(x)^{\top} d + \frac{L}{2} ||d||^{3} \le \alpha \nabla f(x)^{\top} d$$

$$\frac{\|d\|^{3}}{|\nabla f(x)^{\mathsf{T}}d|} \le \frac{1 - 2\alpha}{L} \qquad \|\nabla f(x)\| \le \frac{(1 - 2\alpha)m^{2}}{L}$$

$$\|\nabla f(x + td)\| \le \frac{L}{2m^{2}} \|\nabla f(x)\|^{2} \qquad \|\nabla f(x + td)\| \le \frac{(1 - \alpha)^{2}m^{2}}{2L} \le \frac{(1 - \alpha)m^{2}}{L}$$

• if for \hat{k} , $\left\|\nabla f(x^{\hat{k}})\right\| \le \frac{(1-2\alpha)m^2}{L} \qquad \left\|\nabla f(x^k)\right\| \le \frac{(1-2\alpha)m^2}{L}, \forall k > \hat{k}$





• for any $k > \hat{k}$

$$\frac{L}{2m^{2}} \|\nabla f(x^{k})\| \le \left(\frac{L}{2m^{2}} \|\nabla f(x^{k})\|^{2}\right)^{2^{k-k}} \le \left(\frac{1}{2}\right)^{2^{k-k}}$$

following the analysis in GD

$$f(x^{k}) - f^{*} \leq \frac{4m^{4}}{C_{1}L^{2}} \left(\frac{1}{2}\right)^{2^{k-k+1}}$$

$$\frac{M^{2}L^{2}/m^{5}}{\alpha\beta\min\{1, 9(1-2\alpha)^{2}\}} (f(x^{(0)}) - p^{*}).$$



$$2^{2^6} \approx 10^{19}$$
 Generally, we only needs no more than 6 iteration in this phase

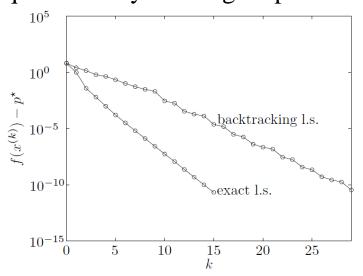


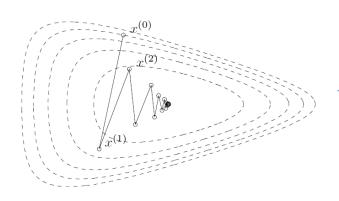
• when $\left\|\nabla f(x^{\hat{k}})\right\| > \frac{(1-2\alpha)m^2}{L} \triangleq \eta$

following the discussion in GD, we will have

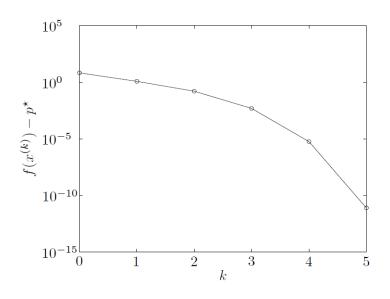
$$f(x^k) - f(x^{k+1}) \ge C\eta^2$$

quadratically convergent phase





before: damped Newton phase



$$f(x_1, x_2) = e^{x_1 + 3x_2 - 0.1} + e^{x_1 - 3x_2 - 0.1} + e^{-x_1 - 0.1}.$$



• when
$$\left\|\nabla f(x^{\hat{k}})\right\| > \frac{(1-2\alpha)m^2}{L} \triangleq \eta$$

following the discussion in GD, we will have

$$x^{(0)}$$

$$x^{(1)}$$

$$f(x^k) - f(x^{k+1}) \ge C\eta^2$$

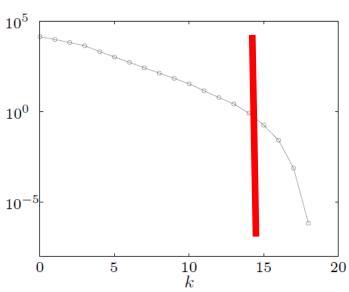


quadratically convergent phase

- Convergence of Newton's method is rapid in general, and quadratic near x^* . Once the quadratic convergence phase is reached, at most six or so iterations are required to produce a solution of very high accuracy.
- Newton's method is affine invariant. It is insensitive to the choice of coordinates, or the condition number of the sublevel sets of the objective.
- Newton's method scales well with problem size. Its performance on problems in \mathbf{R}^{10000} is similar to its performance on problems in \mathbf{R}^{10} , with only a modest increase in the number of steps required.
- The good performance of Newton's method is not dependent on the choice of algorithm parameters. In contrast, the choice of norm for steepest descent plays a critical role in its performance.

$$f(x) = -\sum_{i=1}^{10000} \log(1 - x_i^2) - \sum_{i=1}^{100000} \log(b_i - a_i^T x)$$

before: damped Newton phase







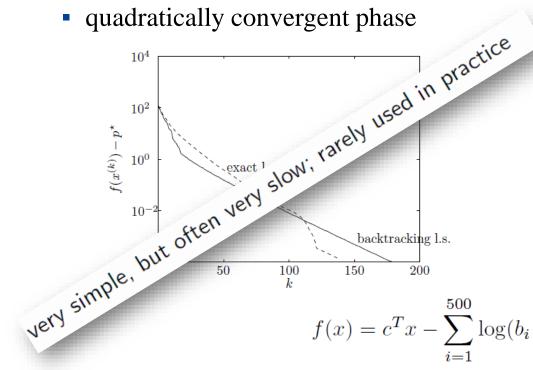
• when $\|\nabla f(x^{\hat{k}})\| > \frac{(1-2\alpha)m^2}{I} \triangleq \eta$

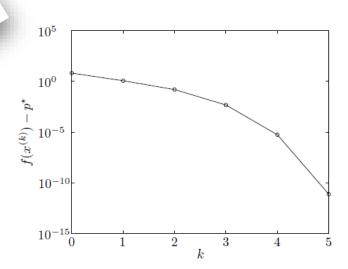
following the discussion in GD, we will have

ag the discussion in GD, we we find
$$f(x^k) - f(x^{k+1}) \ge C\eta^2$$

before: damped Newton phase

quadratically convergent phase





$$f(x) = c^T x - \sum_{i=1}^{500} \log(b_i - a_i^T x)$$

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Comparison: GD and Newton's Method_

gradient descent

$$f(x^k) - f^* \le (1 - c)^k (f(x^{(0)}) - f^*)$$

- linear convergence: stairwise
- affine variant: line search is helpful
- cheap for calculation
- Newton's method

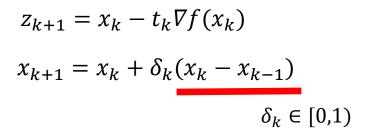
$$f(x^k) - f^* \le \frac{4m^4}{C_1 L^2} \left(\frac{1}{2}\right)^{2^{k-k+1}}$$

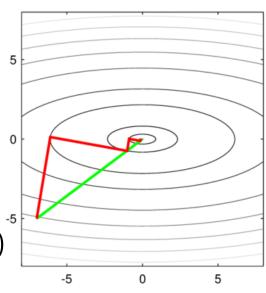
- two phases
- affine invariant: full step could be used
- expensive: the inverse of the Hessian
- can we have something between gradient descent and Newton's method
 - acceptable additional computation to estimate second-order information

Momentum could help



- estimate the second-order information by several gradient
- **=**
- Hessian: the change (gradient) of gradient
- $\nabla f(x^k) \approx \nabla f(x^{k-1}) + t\nabla^2 f(x^{k-1})$ we can assume it is unchanged
- gradient descent may have stairwise phenomena
 - calculating the current direction needs to consider about earlier steps
 - $\nabla f(x^{k+1})$ is different to $\nabla f(x^k)$ and similar to $\nabla f(x^{k-1})$
- using momentum information to lookahead gradient







Polyak's momentum



- using momentum information to lookahead gradient
- Polyak's momentum algorithm

$$x_{k+1} = x_k - t_k \nabla f(x_k) + \delta_k (x_k - x_{k-1}) \quad \rightleftharpoons$$

$$f(x) = \frac{1}{2}x^{\mathsf{T}}Sx$$
 $\nabla f(x) = Sx$

$$x_{k+1} = x_k - t_k z_k$$

$$z_k = \nabla f(x_k) + \beta_k z_{k-1}$$

$$x_{k+1} = x_k - t_k z_k$$

$$z_{k+1} - S x_{k+1} = \beta_k z_k$$

$$\begin{bmatrix} 1 & 0 \\ -S & 1 \end{bmatrix} \begin{bmatrix} x_{k+1} \\ z_{k+1} \end{bmatrix} = \begin{bmatrix} 1 & -t_k \\ 0 & \boldsymbol{\beta_k} \end{bmatrix} \begin{bmatrix} x_k \\ z_k \end{bmatrix}$$

$$Sq = \lambda q \qquad x_k = c_k q$$

$$\nabla f(x) = Sx_k = c_k \lambda q \qquad z_k = d_k q$$

$$\begin{bmatrix} c_{k+1} \\ d_{k+1} \end{bmatrix} = \begin{bmatrix} 1 & -t_k \\ \lambda & \beta_k - \lambda \end{bmatrix} \begin{bmatrix} c_k \\ d_k \end{bmatrix} \quad \longleftarrow \quad \begin{bmatrix} 1 & 0 \\ -\lambda & 1 \end{bmatrix} \begin{bmatrix} c_{k+1} \\ d_{k+1} \end{bmatrix} = \begin{bmatrix} 1 & -t_k \\ 0 & \beta_k \end{bmatrix} \begin{bmatrix} c_k \\ d_k \end{bmatrix}$$

R we can choose t_k and β_k to make R small



Polyak's momentum

- choose t_k and β_k to make R, the eigenvalue e_1 , e_2 , small
- $R = \begin{bmatrix} 1 & -t_k \\ \lambda & \beta_k \lambda \end{bmatrix}$ is dependent on λ : $m \le \lambda \le M$ $f(x^{(k)}) p^* \le (1 m/M)^k (f(x^{(0)}) p^*)$ gradient descent

$$\min_{\beta,t} \sup_{m \leq \lambda \leq M} \max\{e_1(\lambda,\beta,t), e_2(\lambda,\beta,t)\}$$

$$t^* = \left(\frac{2}{\sqrt{M} + \sqrt{m}}\right)^2 \qquad \beta^* = \left(\frac{\sqrt{M} - \sqrt{m}}{\sqrt{M} + \sqrt{m}}\right)^2$$

"miracles do not happen so much in math"

—— Gilbert Strang

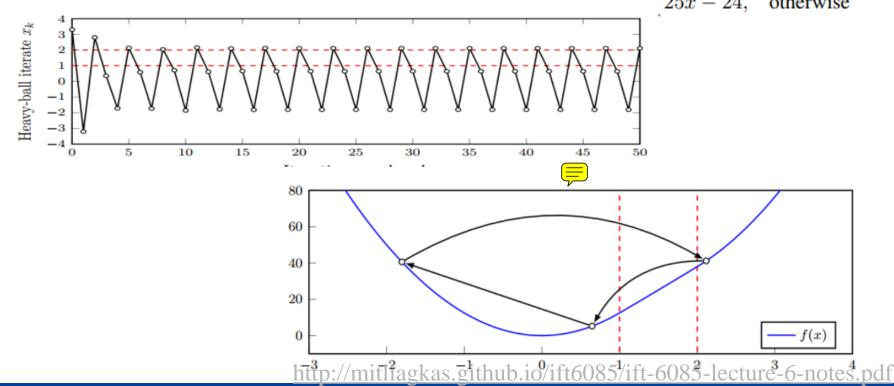


Polyak's momentum



- using momentum information to lookahead gradient
- Polyak's momentum algorithm

$$x_{k+1} = x_k - t_k \nabla f(x_k) + \delta_k(x_k - x_{k-1}) \qquad \nabla f(x) = \begin{cases} 25x, & \text{if } x < 1 \\ x + 24, & \text{if } 1 \le x < 2 \\ 25x - 24, & \text{otherwise} \end{cases}$$





Nesterov Acceleration



• Polyak's momentum algorithm $x_{k+1} = x_k - t_k \nabla f(x_k) + \delta_k (x_k - x_{k-1})$ $z_{k+1} = x_k - t_k \nabla f(x_k)$

$$x_{k+1} = x_k + \delta_k(x_k - x_{k-1})$$
 $\delta_k \in [0,1)$

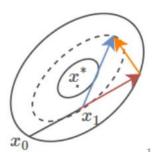
• Nesterov acceleration $x_{k+1} \approx x_k - t_k \nabla f(x_k + \delta_k(x_k - x_{k-1})) + \delta_k(x^k - x^{k-1})$

$$z_{k+1} = x_k - t_k \nabla f(x_k)$$

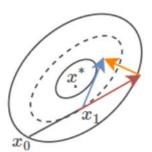
$$x_{k+1} = z_{k+1} + \delta_k(z_{k+1} - z_k)$$
 $\delta_k \in [0,1)$



Polyak's Momentum



Nesterov Momentum



evaluates the gradient after applying momentum

http://mitliagkas.github.io/ift6085/ift-6085-lecture-6-notes.pdf

Nesterov Acceleration



- Polyak's momentum algorithm $x_{k+1} = x_k t_k \nabla f(x_k) + \delta_k (x_k x_{k-1})$ $z_{k+1} = x_k - t_k \nabla f(x_k)$ $x_{k+1} = x_k + \delta_k (x_k - x_{k-1})$ $\delta_k \in [0,1)$
- Nesterov acceleration $x_{k+1} \approx x_k t_k \nabla f(x_k + \delta_k(x_k x_{k-1})) + \delta_k(x^k x^{k-1})$ $z_{k+1} = x_k t_k \nabla f(x_k)$ $x_{k+1} = z_{k+1} + \delta_k(z_{k+1} z_k) \quad \delta_k \in [0,1)$
- accelerated gradient descent can be viewed as:
 - a linear coupling of gradient descent and mirror descent (primal-dual)
 - a discretization of a certain second-order ODE https://arxiv.org/abs/1407.1537

https://arxiv.org/abs/1503.01243



Nesterov Acceleration



Nesterov acceleration

$$y^{k+1} = x^k - \gamma^k \nabla f(x^k)$$

$$x^{k+1} = y^{k+1} + \mu^k (y^{k+1} - y^k) \quad \mu^k \in [0,1)$$

$$t^{k+1} = \frac{1 + \sqrt{1 + 4t_k}}{2}, \qquad \mu^k = \frac{t^k - 1}{t^{k+1}}$$

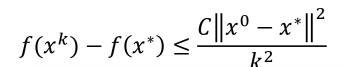


Table 1: Convergence rate for Gradient Descent & Nesterov Accelerated Gradient

Class of Function	GD	NAG
Smooth	O(1/T)	$O(1/T^2)$
Smooth & Strongly-Convex	$O\left(exp\left(-\frac{T}{\kappa}\right)\right)$	$O\left(exp\left(-\frac{T}{\sqrt{\kappa}}\right)\right)$



Fast ISTA

A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems*

Amir Beck† and Marc Teboulle

$$\min_{x} \ \lambda \|x\|_{1} + \|Ax - B\|_{2}^{2}$$



ISTA

$$x^{k+1} = S_{\lambda} \left(x^{k} - A^{\mathsf{T}} (Ax^{k} - B) \right)$$

$$S_{\lambda} = \underset{\mathbf{x}}{\operatorname{argmin}} \left\{ g(\mathbf{x}) + \frac{L}{2} \| \mathbf{x}_{\text{blo}} \left(\mathbf{y}_{\text{div}} - \frac{1}{L} \nabla f(\mathbf{y}) \right) \|^{2} \right\}$$

FISTA

$$y^{k+1} = S_{\lambda} \left(x^k - A^{\mathsf{T}} (B - A x^k) \right)$$
$$t^{k+1} = \frac{1 + \sqrt{1 + 4t_k}}{2}$$
$$x^{k+1} = y^{k+1} + \left(\frac{t^k - 1}{t^{k+1}} \right) (y^{k+1} - y^k)$$



Fast ISTA

A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems*

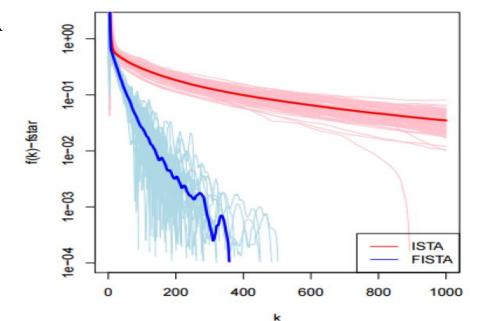
Amir Beck† and Marc Teboulle‡

$$\min_{x} \ \lambda \|x\|_{1} + \|Ax - B\|_{2}^{2}$$

ISTA

$$x^{k+1} = S_{\lambda} (x^k - A^{\mathsf{T}} (Ax^k - B))$$

• FISTA





Home Work



- If your problem is a non-constrained problem
 - implement gradient descent and accelerate it by Nestrov method. Submit the code and draw the convergence curves: (1) $f(x^k)$ v. s. k and (a) $f(x^k)$ v. s. time
- If your problem is a constrained one
 - 9.10 (please submit your code as well)

THANKS



Lemmas



$$\begin{split} f\big(x-t\nabla f(x)\big)-f(y) &\leq f\big(x-t\nabla f(x)\big)-f(x)+\nabla f(x)^{\top}(x-y)\\ &\leq \nabla f(x)^{\top}(x-t\nabla f(x)-x)+\frac{1}{2t}\|x-t\nabla f(x)-x\|^2+\nabla f(x)^{\top}(x-y)\\ &=-\frac{t}{2}\|\nabla f(x)\|^2+\nabla f(x)^{\top}(x-y) \end{split}$$



$y^{k+1} = x^k - \gamma^k \nabla f(x^k)$

$$f(y^{k+1}) - f(y^k) = f\left(x^k - t\nabla f(x^k)\right) - f(y^k) \le -\frac{t}{2} \|\nabla f(x^k)\|^2 + \nabla f(x^k)^{\mathsf{T}} (x^k - y^k)$$

$$= -\frac{1}{2t} \|y^{k+1} - x^k\|^2 - \frac{1}{t} (y^{k+1} - x^k)^{\mathsf{T}} (x^k - y^k)$$

$$f(y^{k+1}) - f(x^*) \le -\frac{1}{2t} \|y^{k+1} - x^k\|^2 - \frac{1}{t} (y^{k+1} - x^k)^{\mathsf{T}} (x^k - x^*)$$

Lemmas



$$\begin{split} f\big(x-t\nabla f(x)\big)-f(y) &\leq f\big(x-t\nabla f(x)\big)-f(x)+\nabla f(x)^\top(x-y)\\ &\leq \nabla f(x)^\top(x-t\nabla f(x)-x)+\frac{1}{2t}\|x-t\nabla f(x)-x\|^2+\nabla f(x)^\top(x-y)\\ &=-\frac{t}{2}\|\nabla f(x)\|^2+\nabla f(x)^\top(x-y) \end{split}$$



$y^{k+1} = x^k - \gamma^k \nabla f(x^k)$

$$\frac{t}{2} \|\nabla f(x^{k})\|^{2} - \nabla f(x^{k})^{\mathsf{T}} (x^{k} - y^{k}) = \frac{\gamma^{k}}{2} \left(\|\nabla f(x^{k})\|^{2} - \frac{2}{\gamma^{k}} \nabla f(x^{k})^{\mathsf{T}} (x^{k} - y^{k}) \right) \\
= \frac{\gamma^{k}}{2} \left(\left\| \nabla f(x^{k}) - \frac{1}{\gamma^{k}} \nabla f(x^{k})^{\mathsf{T}} (x^{k} - y^{k}) \right\|^{2} - \frac{1}{\gamma^{k^{2}}} \|x^{k} - y^{k}\|^{2} \right) \\
= \frac{\gamma^{k}}{2} \left(\frac{1}{\gamma^{k^{2}}} \|y^{k} - (x^{k} - \gamma^{k} \nabla f(x^{k}))\|^{2} - \frac{1}{\gamma^{k^{2}}} \|x^{k} - y^{k}\|^{2} \right) \\
f(y^{k+1}) - f(y^{k}) \leq \frac{1}{2t} \left(\|y - (x - \alpha \nabla f(x))\|^{2} - \|x^{k} - y^{k}\|^{2} \right)$$

Convergence Analysis

$$y_{k+1} = x_k - t_k \nabla f(x_k)$$
 $x_{k+1} = z_{k+1} + \delta_k (y_{k+1} - y_k)$ $\delta_k \in [0,1)$

$$f(x - t\nabla f(x)) - f(y) \le f(x - t\nabla f(x)) - f(x) + \nabla f(x)^{\mathsf{T}}(x - y)$$

$$\le \nabla f(x)^{\mathsf{T}}(x - t\nabla f(x) - x) + \frac{1}{2t} \|x - t\nabla f(x) - x\|^2 + \nabla f(x)^{\mathsf{T}}(x - y)$$

$$= -\frac{t}{2} \|\nabla f(x)\|^2 + \nabla f(x)^{\mathsf{T}}(x - y)$$

$$f(y^{k+1}) - f(y^k) = f(x^k - t\nabla f(x^k)) - f(y^k) \le -\frac{t}{2} \|\nabla f(x^k)\|^2 + \nabla f(x^k)^{\mathsf{T}} (x^k - y^k)$$
$$= -\frac{1}{2t} \|y^{k+1} - y^k\|^2 - \frac{1}{t} (y^{k+1} - y^k)^{\mathsf{T}} (x^k - y^k)$$

$$f(y^{k+1}) - f(x^*) \le -\frac{1}{2t} \|y^{k+1} - y^k\|^2 - \frac{1}{t} (y^{k+1} - y^k)^{\mathsf{T}} (x^k - x^*)$$