# **Proximal Gradient Method**

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#### Outline

- A fundamental inequality
- Nonconvex setting
- Convex setting
- Strongly convex setting
- Backtracking
- Stopping conditions
- Accelerated gradient method
- Scaling

#### Proximal gradient method

We consider composite optimization problems of the form

$$\underset{x}{\text{minimize}} f(x) + g(x)$$

The proximal gradient method is

$$\begin{aligned} x_{k+1} &= \operatorname*{argmin}_{y} \left( f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2\gamma_k} \|y - x_k\|_2^2 + g(y) \right) \\ &= \operatorname*{argmin}_{y} \left( g(y) + \frac{1}{2\gamma_k} \|y - (x_k - \gamma_k \nabla f(x_k))\|_2^2 \right) \\ &= \operatorname*{prox}_{\gamma_k g} (x_k - \gamma_k \nabla f(x_k)) \end{aligned}$$

# Proximal gradient - Optimality condition

Proximal gradient iteration is:

$$x_{k+1} = \operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

$$= \underset{y}{\operatorname{argmin}} (g(y) + \underbrace{\frac{1}{2\gamma_k} \|y - (x_k - \gamma_k \nabla f(x_k))\|_2^2}_{h(y)})$$

where  $x_{k+1}$  is unique due to strong convexity of h

ullet Fermat's rule gives, since g convex, optimality condition:

$$0 \in \partial g(x_{k+1}) + \partial h(x_{k+1})$$
  
=  $\partial g(x_{k+1}) + \gamma_k^{-1}(x_{k+1} - (x_k - \gamma_k \nabla f(x_k)))$ 

since h differentiable

• A consequence is that  $\partial g(x_{k+1})$  is nonempty

# Proximal gradient method – Convergence rates

- We will analyze proximal gradient method in different settings:
  - Nonconvex
    - ullet O(1/k) convergence for squared residual
  - Convex
    - O(1/k) convergence for function values
  - Strongly convex
    - Linear convergence in distance to solution
- First two rates based on a fundamental inequality for the method

# Assumptions for fundamental inequality

- (i)  $f:\mathbb{R}^n \to \mathbb{R}$  is continuously differentiable (not necessarily convex)
- (ii) For every  $x_k$  and  $x_{k+1}$  there exists  $\beta_k \in [\eta, \eta^{-1}]$ ,  $\eta \in (0, 1]$ :

$$f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_k - x_{k+1}||_2^2$$

where  $\beta_k$  is a sort of local Lipschitz constant

- $(iii) \ g: \mathbb{R}^n o \mathbb{R} \cup \{\infty\}$  is closed convex
- (iv) A minimizer  $x^\star$  exists and  $p^\star = f(x^\star) + g(x^\star)$  is optimal value
  - (v) Proximal gradient method parameters  $\gamma_k > 0$

- Assumption (ii) satisfied with  $\beta_k \geq \beta$  if f is  $\beta$ -smooth
- Assumptions will be strengthened later

# A fundamental inequality

For all  $z \in \mathbb{R}^n$ , the proximal gradient method satisfies

$$f(x_{k+1}) + g(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (z - x_k) - \frac{\gamma_k^{-1} - \beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z) + \frac{1}{2\gamma_k} (||x_k - z||_2^2 - ||x_{k+1} - z||_2^2)$$

where 
$$x_{k+1} = \operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

# A fundamental inequality – Proof (1/2)

Using

- (a) Upper bound assumption on f, i.e., Assumption (ii)
- (b) Prox optimality condition: There exists  $s_{k+1} \in \partial g(x_{k+1})$

$$0 = s_{k+1} + \gamma_k^{-1}(x_{k+1} - (x_k - \gamma_k \nabla f(x_k)))$$

(c) Subgradient definition:  $\forall z, g(z) \geq g(x_{k+1}) + s_{k+1}^T(z - x_{k+1})$ 

$$f(x_{k+1}) + g(x_{k+1})$$

$$\stackrel{(a)}{\leq} f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(x_{k+1})$$

$$\stackrel{(c)}{\leq} f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z)$$

$$- s_{k+1}^T (z - x_{k+1})$$

$$\stackrel{(b)}{=} f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z)$$

$$+ \gamma_k^{-1} (x_{k+1} - (x_k - \gamma_k \nabla f(x_k)))^T (z - x_{k+1})$$

$$= f(x_k) + \nabla f(x_k)^T (z - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z)$$

$$+ \gamma_k^{-1} (x_{k+1} - x_k)^T (z - x_{k+1})$$

# A fundamental inequality – Proof (2/2)

The proof continues by using the equality

$$(x_{k+1} - x_k)^T (z - x_{k+1})$$

$$= \frac{1}{2} (\|x_k - z\|_2^2 - \|x_{k+1} - z\|_2^2 - \|x_{k+1} - x_k\|_2^2)$$

Applying to previous inequality gives

$$f(x_{k+1}) + g(x_{k+1})$$

$$\leq f(x_k) + \nabla f(x_k)^T (z - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z)$$

$$+ \gamma_k^{-1} (x_{k+1} - x_k)^T (z - x_{k+1})$$

$$= f(x_k) + \nabla f(x_k)^T (z - x_k) + \frac{\beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z)$$

$$+ \frac{1}{2\gamma_k} (||x_k - z||_2^2 - ||x_{k+1} - z||_2^2 - ||x_k - x_{k+1}||_2^2)$$

which after rearrangement gives the fundamental inequality

#### Outline

- A fundamental inequality
- Nonconvex setting
- Convex setting
- Strongly convex setting
- Backtracking
- Stopping conditions
- Accelerated gradient method
- Scaling

# Nonconvex setting

We will analyze the proximal gradient method

$$x_{k+1} = \text{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

in a nonconvex setting for solving

minimize 
$$f(x) + g(x)$$

- Will show sublinear O(1/k) convergence
- Analysis based on *A fundamental inequality*

# Nonconvex setting – Assumptions

- (i)  $f: \mathbb{R}^n \to \mathbb{R}$  is continuously differentiable (not necessarily convex)
- (ii) For every  $x_k$  and  $x_{k+1}$  there exists  $\beta_k \in [\eta, \eta^{-1}]$ ,  $\eta \in (0, 1]$ :

$$f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_k - x_{k+1}||_2^2$$

where  $\beta_k$  is a sort of local Lipschitz constant

- (iii)  $g: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$  is closed convex
- (iv) A minimizer  $x^\star$  exists and  $p^\star = f(x^\star) + g(x^\star)$  is optimal value
  - (v) Algorithm parameters  $\gamma_k \in [\epsilon, \frac{2}{\beta_k} \epsilon]$ , where  $\epsilon > 0$

- Differs from assumptions for fundamental inequality only in (v)
- Assumption (ii) satisfied with  $\beta_k \geq \beta$  if f is  $\beta$ -smooth

# Nonconvex setting – Analysis

• Use fundamental inequality

$$f(x_{k+1}) + g(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (z - x_k) - \frac{\gamma_k^{-1} - \beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(z) + \frac{1}{2\gamma_k} (||x_k - z||_2^2 - ||x_{k+1} - z||_2^2)$$

• Set  $z = x_k$  to get

$$f(x_{k+1}) + g(x_{k+1}) \le f(x_k) + g(x_k) - (\gamma_k^{-1} - \frac{\beta_k}{2}) ||x_{k+1} - x_k||_2^2$$

#### **Step-size requirements**

• Step-sizes  $\gamma_k$  should be restricted for inequality to be useful:

$$f(x_{k+1}) + g(x_{k+1}) \le f(x_k) + g(x_k) - (\gamma_k^{-1} - \frac{\beta_k}{2}) ||x_{k+1} - x_k||_2^2$$

- Requirements  $\beta_k \in [\eta, \eta^{-1}]$  and  $\gamma_k \in [\epsilon, \frac{2}{\beta_k} \epsilon]$ :
  - upper bound  $\gamma_k \leq \frac{2}{\beta_k} \epsilon$  can be written as

$$\gamma_k \le \frac{2}{\beta_k + 2\delta_k}$$
 where  $\delta_k = \frac{\beta_k \epsilon}{2\left(\frac{2}{\beta_k} - \epsilon\right)} \ge \frac{\beta_k^2 \epsilon}{4} \ge \frac{\eta^2 \epsilon}{4} > 0$ 

since upper bound  $\beta_k \leq \eta^{-1}$  gives  $\frac{2}{\beta_k} - \epsilon \geq 2\eta - \epsilon > 0$  and  $\epsilon > 0$ 

• Inverting upper step-size bound and letting  $\delta:=\frac{\eta^2\epsilon}{4}\leq \delta_k$ :

$$\gamma_k^{-1} \ge \frac{\beta_k + 2\delta_k}{2} \ge \frac{\beta_k}{2} + \delta \qquad \Rightarrow \qquad \gamma_k^{-1} - \frac{\beta_k}{2} \ge \delta > 0$$

• This implies, by subtracting  $p^{\star}$  from both sides to have  $V_k \geq 0$ ,

$$\underbrace{f(x_{k+1}) + g(x_{k+1}) - p^{\star}}_{V_{k+1}} \le \underbrace{f(x_k) + g(x_k) - p^{\star}}_{V_k} - \underbrace{\delta ||x_{k+1} - x_k||_2^2}_{R_k}$$

where bounds on  $\gamma_k$  imply that all  $R_k$  are nonnegative

#### Lyapunov inequality consequences

Restating Lyapunov inequality

$$\underbrace{f(x_{k+1}) + g(x_{k+1}) - p^*}_{V_{k+1}} \le \underbrace{f(x_k) + g(x_k) - p^*}_{V_k} - \underbrace{\delta ||x_{k+1} - x_k||_2^2}_{R_k}$$

- Consequences:
  - Function value is decreasing sequence (may not converge to  $p^*$ )
  - Fixed-point residual converges to 0 as  $k \to \infty$ :

$$||x_{k+1} - x_k||_2 = ||\operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k)) - x_k||_2 \to 0$$

• Best fixed-point residual norm square converges as O(1/k):

$$\min_{i \in \{0, \dots, k\}} \|x_{i+1} - x_i\|_2^2 \le \frac{f(x_0) + g(x_0) - p^*}{\delta(k+1)}$$

# Lyapunov inequality consequences – g = 0

• For g=0, then  $x_{k+1}=x_k-\gamma_k\nabla f(x_k)$  and

$$||x_{k+1} - x_k||_2 = \gamma_k ||\nabla f(x_k)||_2$$
 and  $R_k = \delta \gamma_k^2 ||\nabla f(x_k)||_2^2$ 

- Lyapunov inequality consequences in this setting:
  - Gradient converges to 0 (since  $\gamma_k \geq \epsilon$ ):  $\|\nabla f(x_k)\|_2 \to 0$
  - Smallest gradient norm square converges as:

$$\min_{i \in \{0, \dots, k\}} \|\nabla f(x_i)\|_2^2 \le \frac{f(x_0) - p^*}{\delta \sum_{i=0}^k \gamma_i^2}$$

• If, in addition, f is  $\beta$ -smooth and  $\gamma_k = \frac{1}{\beta}$ :

$$\min_{i \in \{0, \dots, k\}} \|\nabla f(x_i)\|_2^2 \le \frac{2\beta(f(x_0) - p^*)}{k+1}$$

since then 
$$\beta_k=\beta$$
 and  $\gamma_k^{-1}-\frac{\beta_k}{2}=\frac{\beta}{2}=\delta>0$ 

So, will approach local maximum, minimum, or saddle-point

# Fixed-point residual convergence – Implication

What does  $\|\operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k)) - x_k\|_2 \to 0$  imply?

• By prox-grad optimality condition and  $||x_{k+1} - x_k||_2 \to 0$ :

$$\partial g(x_{k+1}) + \nabla f(x_k) \ni \gamma_k^{-1}(x_k - x_{k+1}) \to 0$$

as  $k \to \infty$  (since  $\gamma_k \ge \epsilon$ , i.e.,  $0 < \gamma_k^{-1} \le \epsilon^{-1}$ ) or equivalently

$$\partial g(x_{k+1}) + \nabla f(x_{k+1}) \ni \underbrace{\gamma_k^{-1}(x_k - x_{k+1}) + \nabla f(x_{k+1}) - \nabla f(x_k)}_{u_k} \to 0$$

where  $u_k \to 0$  is concluded by continuity of  $\nabla f$ 

Critical point definition for nonconvex f satisfied in the limit

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#### **Convex setting**

We will analyze the proximal gradient method

$$x_{k+1} = \text{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

in the convex setting for solving

minimize 
$$f(x) + g(x)$$

- ullet Will show sublinear O(1/k) convergence for function values
- Analysis based on A fundamental inequality

# **Convex setting – Assumptions**

- (i)  $f: \mathbb{R}^n \to \mathbb{R}$  is continuously differentiable and convex
- (ii) For every  $x_k$  and  $x_{k+1}$  there exists  $\beta_k \in [\eta, \eta^{-1}]$ ,  $\eta \in (0, 1]$ :

$$f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_k - x_{k+1}||_2^2$$

where  $\beta_k$  is a sort of local Lipschitz constant

- (iii)  $g: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$  is closed convex
- (iv) A minimizer  $x^\star$  exists and  $p^\star = f(x^\star) + g(x^\star)$  is optimal value
  - (v) Algorithm parameters  $\gamma_k \in [\epsilon, \frac{2}{\beta_k} \epsilon]$ , where  $\epsilon > 0$

- Assumptions as for fundamental inequality plus
  - convexity of f
  - ullet restricted step-size parameters  $\gamma_k$  (as in nonconvex setting)
- Assumption (ii) satisfied with  $\beta_k \geq \beta$  if f is  $\beta$ -smooth

#### Convex setting - Analysis

• Use fundamental inequality with  $z=x^{\star}$ , where  $x^{\star}$  is solution

$$f(x_{k+1}) + g(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x^* - x_k)$$
$$- \frac{\gamma_k^{-1} - \beta_k}{2} ||x_{k+1} - x_k||_2^2 + g(x^*)$$
$$+ \frac{1}{2\gamma_k} (||x_k - x^*||_2^2 - ||x_{k+1} - x^*||_2^2)$$

and convexity of f

$$f(x^*) \ge f(x_k) + \nabla f(x_k)^T (x^* - x_k)$$

• This gives

$$f(x_{k+1}) + g(x_{k+1}) \le f(x^*) - \frac{\gamma_k^{-1} - \beta_k}{2} \|x_{k+1} - x_k\|_2^2 + g(x^*) + \frac{1}{2\gamma_k} (\|x_k - x^*\|_2^2 - \|x_{k+1} - x^*\|_2^2)$$

which, by multiplying by  $2\gamma_k$  and using  $p^* = f(x^*) + g(x^*)$ , gives

$$||x_{k+1} - x^*||_2^2 \le ||x_k - x^*||_2^2 + (\beta_k \gamma_k - 1)||x_{k+1} - x_k||_2^2$$
$$-2\gamma_k (f(x_{k+1}) + g(x_{k+1}) - p^*)$$

#### **Lyapunov inequality – Convex setting**

The last inequality on previous slide is Lyapunov inequality

$$\underbrace{\|x_{k+1} - x^*\|_{2}^{2}}_{V_{k+1}} \le \underbrace{\|x_{k} - x^*\|_{2}^{2}}_{V_{k}} + \underbrace{(\beta_{k}\gamma_{k} - 1)\|x_{k+1} - x_{k}\|_{2}^{2}}_{W_{k}} - 2\gamma_{k}\underbrace{(f(x_{k+1}) + g(x_{k+1}) - p^*)}_{R}$$

- Will divide analysis two cases: Short and long step-sizes
  - Step-sizes  $\gamma_k \in [\epsilon, \frac{1}{\beta_k}]$ : gives  $\beta_k \gamma_k \leq 1$  and  $W_k \leq 0$
  - Step-sizes  $\gamma_k \in [\frac{1}{\beta_k}, \frac{2}{\beta_k} \epsilon]$ : gives  $\beta_k \gamma_k \ge 1$  and  $W_k \ge 0$  since  $W_k$  contribute differently

#### Short step-sizes

• For step-sizes  $\gamma_k \in [\epsilon, \frac{1}{\beta_k}]$ , the Lyapunov inequality implies:

$$\underbrace{\|x_{k+1} - x^*\|_2^2}_{V_{k+1}} \le \underbrace{\|x_k - x^*\|_2^2}_{V_k} - 2\gamma_k \underbrace{(f(x_{k+1}) + g(x_{k+1}) - p^*)}_{R_k}$$

where we have used  $W_k = 0$  (which is OK since  $W_k \leq 0$ )

- Nonconvex analysis says function value decreases in every iteration
- Consequences:
  - Distance to solution  $||x_k x^*||_2$  converges as  $k \to \infty$
  - Function value decreases to optimal function value as:

$$f(x_{k+1}) + g(x_{k+1}) - p^* \le \frac{\|x_0 - x^*\|_2^2}{2\sum_{i=0}^k \gamma_i}$$

if f is  $\beta$ -smooth and  $\gamma_k = \frac{1}{\beta}$ , then converges as O(1/k):

$$f(x_{k+1}) + g(x_{k+1}) - p^* \le \frac{\beta ||x_0 - x^*||_2^2}{2(k+1)}$$

#### Long step-sizes

• For step-sizes  $\gamma_k \in [\frac{1}{\beta_k}, \frac{2}{\beta_k} - \epsilon]$ , the Lyapunov inequality is:

$$\underbrace{\frac{\|x_{k+1} - x^*\|_2^2}{V_{k+1}}} \leq \underbrace{\frac{\|x_k - x^*\|_2^2}{V_k} + \underbrace{(\beta_k \gamma_k - 1) \|x_{k+1} - x_k\|_2^2}_{W_k} - 2\gamma_k \underbrace{(f(x_{k+1}) + g(x_{k+1}) - p^*)}_{R_k}$$

- From nonconvex analysis can conclude that  $W_k$  is summable
  - We showed for  $\gamma_k \in [\epsilon, \frac{2}{\beta_k} \epsilon]$ ,  $(\|x_{k+1} x_k\|_2^2)_{k \in \mathbb{N}}$  is summable
  - Since  $\beta_k \gamma_k$  bounded, also  $(W_k)_{k \in \mathbb{N}}$  is summable
  - Let us define  $\overline{W} = \sum_{k=0}^{\infty} W_k$
- Consequences:
  - Distance to solution  $||x_k x^*||_2$  converges as  $k \to \infty$
  - Function value decreases to optimal function value as:

$$f(x_{k+1}) + g(x_{k+1}) - p^* \le \frac{\|x_0 - x^*\|_2^2 + \overline{W}}{2\sum_{i=0}^k \gamma_i}$$

for  $\beta\text{-smooth }f$  with  $\gamma_k=\frac{1}{\beta}\text{, denominator replaced by }\frac{2(k+1)}{\beta}$ 

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# Strongly convex setting

We will analyze the proximal gradient method

$$x_{k+1} = \operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

in a strongly convex setting for solving

$$minimize f(x) + g(x)$$

- Will show linear convergence for distance to solution  $||x_k x^*||_2$
- Two ways to show linear convergence, we can:
  - (i) Base analysis on A fundamental inequality
  - (ii) Start by  $||x_{k+1} x^*||_2^2$  and expand (which is what we will do)

# Strongly convex setting – Assumptions

- (i)  $f:\mathbb{R}^n \to \mathbb{R}$  is continuously differentiable and  $\sigma$ -strongly convex
- (ii) f is  $\beta$ -smooth
- $(iii) \ g: \mathbb{R}^n o \mathbb{R} \cup \{\infty\}$  is closed convex

- Assumptions as for fundamental inequality plus
  - $\sigma$ -strong convexity of f
  - $\beta$ -smoothness of f instead of upper bound for  $x_{k+1}$  and  $x_k$
  - restricted step-size parameters  $\gamma_k$  (as in (non)convex setting)
- But will not use fundamental inequality in analysis

# Strongly convex setting - Analysis

Use that

(a) 
$$x^* = \text{prox}_{\gamma a}(x^* - \gamma \nabla f(x^*))$$
 for all  $\gamma > 0$ 

- (b) the proximal operator is nonexpansive
- (c) gradients of  $\beta$ -smooth  $\sigma$ -strongly convex functions f satisfy

$$(\nabla f(x) - \nabla f(y))^T (x - y) \ge \frac{1}{\beta + \sigma} \|\nabla f(x) - \nabla f(y)\|_2^2 + \frac{\sigma \beta}{\beta + \sigma} \|x - y\|_2^2$$

to get

$$\begin{aligned} &\|x_{k+1} - x^*\|_2^2 \\ &\stackrel{(a)}{=} \|\operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k)) - \operatorname{prox}_{\gamma_k g}(x^* - \gamma_k \nabla f(x^*))\|_2^2 \\ &\stackrel{(b)}{\leq} \|(x_k - \gamma_k \nabla f(x_k)) - (x^* - \gamma_k \nabla f(x^*))\|_2^2 \\ &= \|x_k - x^*\|_2^2 - 2\gamma_k (\nabla f(x_k) - \nabla f(x^*))^T (x_k - x^*) \\ &+ \gamma_k^2 \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \\ &\stackrel{(c)}{\leq} \|x_k - x^*\|_2^2 - \frac{2\gamma_k}{\beta + \sigma} (\|\nabla f(x_k) - \nabla f(x^*)\|_2^2 + \sigma\beta \|x_k - x^*\|_2^2) \\ &+ \gamma_k^2 \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \\ &= (1 - \frac{2\gamma_k \sigma\beta}{\beta + \sigma}) \|x_k - x^*\|_2^2 - \gamma_k (\frac{2}{\beta + \sigma} - \gamma_k) \|\nabla f(x_k) - \nabla f(x^*)\|_2^2 \end{aligned}$$

# Lyapunov inequality – Strongly convex setting

Lyapunov inequality from previous slide is

$$||x_{k+1} - x^*||_2^2 \le (1 - \frac{2\gamma_k \sigma \beta}{\beta + \sigma}) ||x_k - x^*||_2^2 - \underbrace{\gamma_k (\frac{2}{\beta + \sigma} - \gamma_k) ||\nabla f(x_k) - \nabla f(x^*)||_2^2}_{W_k}$$

- Will divide analysis into two cases: Short and long step-sizes
  - Step-sizes  $\gamma_k \in [\epsilon, \frac{2}{\beta + \sigma}]$ : gives  $W_k \geq 0$
  - Step-sizes  $\gamma_k \in [\frac{2}{\beta+\sigma}, \frac{2}{\beta} \epsilon]$ : gives  $W_k \leq 0$

#### Short step-sizes

Lyapunov inequality

$$||x_{k+1} - x^*||_2^2 \le (1 - \frac{2\gamma_k \sigma\beta}{\beta + \sigma}) ||x_k - x^*||_2^2 - \underbrace{\gamma_k (\frac{2}{\beta + \sigma} - \gamma_k) ||\nabla f(x_k) - \nabla f(x^*)||_2^2}_{W_k}$$

for  $\gamma_k \in [\epsilon, \frac{2}{\beta + \sigma}]$  implies  $W_k \geq 0$ 

• Strong monotonicity with modulus  $\sigma$  of  $\nabla f$  implies

$$\|\nabla f(x_k) - \nabla f(x^*)\|_2 \ge \sigma \|x_k - x^*\|_2$$

So we have linear convergence since

$$||x_{k+1} - x^*||_2^2 \le (1 - \frac{2\gamma_k \sigma \beta}{\beta + \sigma} - \sigma^2 \gamma_k (\frac{2}{\beta + \sigma} - \gamma_k)) ||x_k - x^*||_2^2$$

$$= (1 - \frac{2\gamma_k \sigma (\beta + \sigma)}{\beta + \sigma} + \sigma^2 \gamma_k^2) ||x_k - x^*||_2^2$$

$$= (1 - \sigma \gamma_k)^2 ||x_k - x^*||_2^2$$

where  $(1 - \sigma \gamma_k)^2 \in [0, 1)$  for full range of  $\gamma_k$ 

#### Long step-sizes

Lyapunov inequality

$$||x_{k+1} - x^*||_2^2 \le (1 - \frac{2\gamma_k \sigma\beta}{\beta + \sigma}) ||x_k - x^*||_2^2 - \underbrace{\gamma_k (\frac{2}{\beta + \sigma} - \gamma_k) ||\nabla f(x_k) - \nabla f(x^*)||_2^2}_{W_k}$$

for  $\gamma_k \in [\frac{2}{\beta+\sigma}, \frac{2}{\beta}-\epsilon]$  implies  $W_k \leq 0$ 

• That f is  $\beta$ -smooth implies  $\nabla f$  is  $\beta$ -Lipschitz continuous:

$$\|\nabla f(x_k) - \nabla f(x^*)\|_2 \le \beta \|x_k - x^*\|_2$$

So we have linear convergence since

$$||x_{k+1} - x^*||_2^2 \le (1 - \frac{2\gamma_k \sigma \beta}{\beta + \sigma} - \beta^2 \gamma_k (\frac{2}{\beta + \sigma} - \gamma_k)) ||x_k - x^*||_2^2$$

$$= (1 - \frac{2\gamma_k \beta(\sigma + \beta)}{\beta + \sigma} + \beta^2 \gamma_k^2) ||x_k - x^*||_2^2$$

$$= (1 - \beta\gamma_k)^2 ||x_k - x^*||_2^2$$

where  $(1 - \beta \gamma_k)^2 \in [0, 1)$  for full range of  $\gamma_k$ 

#### Unified rate

- By removing the square and checking sign, we have
  - for step-sizes  $\gamma_k \in [\epsilon, \frac{2}{\beta + \sigma}]$ :

$$||x_{k+1} - x^*||_2 \le (1 - \sigma \gamma_k) ||x_k - x^*||_2$$

• for step-sizes  $\gamma_k \in \left[\frac{2}{\beta+\sigma}, \frac{2}{\beta} - \epsilon\right]$ :

$$||x_{k+1} - x^*||_2 \le (\beta \gamma_k - 1)||x_k - x^*||_2$$

• The linear convergence result can be summarized as

$$||x_{k+1} - x^*||_2 \le \max(1 - \sigma \gamma_k, \beta \gamma_k - 1)||x_k - x^*||_2$$

#### Optimal step-size

• For fixed-step-sizes  $\gamma_k = \gamma$ , the rate result is

$$||x_{k+1} - x^*||_2 \le \underbrace{\max(1 - \sigma \gamma, \beta \gamma - 1)}_{\rho} ||x_k - x^*||_2$$

- Optimal  $\gamma$  that gives smallest contraction is  $\gamma = \frac{2}{\beta + \sigma}$ :
  - $(1-\sigma\gamma)$  decreasing in  $\gamma$ , optimal at upper bound  $\gamma=\frac{2}{\beta+\sigma}$   $(\beta\gamma-1)$  increasing in  $\gamma$ , optimal at lower bound  $\gamma=\frac{2}{\beta+\sigma}$

  - Bounds coincide at  $\gamma = \frac{2}{\beta + \sigma}$  to give rate factor  $\rho = \frac{\beta \sigma}{\beta + \sigma}$

#### Outline

- A fundamental inequality
- Nonconvex setting
- Convex setting
- Strongly convex setting
- Backtracking
- Stopping conditions
- Accelerated gradient method
- Scaling

#### Choose $\beta_k$ and $\gamma_k$

• In nonconvex and convex analysis, we assume  $\beta_k$  known such that

$$f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} - x_k) + \frac{\beta_k}{2} ||x_k - x_{k+1}||_2^2$$

for consecutive iterates  $x_k$  and  $x_{k+1}$ 

- ullet This is an assumption on the function f
- We call it descent condition (DC)
- If f is  $\beta$ -smooth, then  $\beta_k = \beta$  is valid choice since

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||_2^2$$

for all x,y, then we can select  $\gamma_k \in [\epsilon, \frac{2}{\beta} - \epsilon]$ 

# Choose $\beta_k$ and $\gamma_k$ – Backtracking

- Larger  $\beta_{k,l_k}$  gives smaller upper bound for step-size  $\gamma_k$
- Forwardtracking on  $\beta_{k,l_k}$ , backtracking for  $\gamma_k$  upper bound

#### When to use backtracking

- f is  $\beta$ -smooth but constant  $\beta$  unknown:
  - initialize  $\beta_{k,0}=\beta_{k-1,\bar{l}_{k-1}}$  to previously used value
  - then  $(\beta_k)_{k\in\mathbb{N}}$  nondecreasing
  - finally  $\beta_k \geq \beta$  (if needed), then
    - step-size bound  $\gamma_k \in [\epsilon, \frac{2}{\beta_{k,\bar{l}_*}} \epsilon]$  makes (DC) hold directly
    - ullet so will have constant  $eta_k$  after finite number of algoritm iterations
- $\nabla f$  locally Lipschitz and sequence bounded (as in convex case):
  - initialize  $\beta_{k,0} = \bar{\beta}$ , for some pre-chosen  $\bar{\beta} > 0$
  - $\bullet$  reset to same value  $\bar{\beta}$  in every algorithm iteration
  - will find a local Lipschitz constant

#### Outline

- A fundamental inequality
- Nonconvex setting
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- Scaling

#### When to stop algorithm?

- Consider minimize f(x) + g(x)
- Apply proximal gradient method  $x_{k+1} = \text{prox}_{\gamma_k q}(x_k \gamma_k \nabla f(x_k))$
- Algorithm sequence satisfies

$$\partial g(x_{k+1}) + \nabla f(x_{k+1}) \ni \underbrace{\gamma_k^{-1}(x_k - x_{k+1}) + \nabla f(x_{k+1}) - \nabla f(x_k)}_{u_k} \to 0$$

is  $||u_k||_2$  small a good measure of being close to fixed-point?

# When to stop algorithm – Scaled problem

Let a > 0 and solve equivalent problem  $\min_{x} \max af(x) + ag(x)$ :

- ullet Denote algorithm parameter  $\gamma_{a,k}=rac{\gamma_k}{a}$
- Algorithm satisfies:

$$x_{k+1} = \operatorname{prox}_{\gamma_{a,k}ag}(x_k - \gamma_{a,k}\nabla af(x_k)) = \operatorname{prox}_{\gamma_k g}(x_k - \gamma_k \nabla f(x_k))$$

i.e., the same algorithm as before

ullet However,  $u_{a,k}$  in this setting satisfies

$$u_{a,k} = \gamma_{a,k}^{-1}(x_k - x_{k+1}) + \nabla a f(x_{k+1}) - \nabla a f(x_k)$$
  
=  $a(\gamma_k^{-1}(x_k - x_{k+1}) + \nabla f(x_{k+1}) - \nabla f(x_k))$   
=  $au_k$ 

i.e., same algorithm but different optimality measure

Optimality measure should be scaling invariant

# Scaling invariant stopping condition

ullet For eta-smooth f, use scaled condition  $\frac{1}{eta}u_k$ 

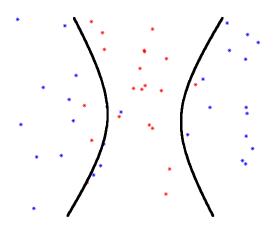
$$\frac{1}{\beta}u_k := \frac{1}{\beta}(\gamma_k^{-1}(x_k - x_{k+1}) + \nabla f(x_{k+1}) - \nabla f(x_k))$$

that we have seen before

- Let us scale problem by a to get minimize af(x) + ag(x), then
  - smoothness constant  $\beta_a=a\beta$  scaled by  $a\Rightarrow$  use  $\gamma_{a,k}=\frac{\gamma_k}{a}$
  - optimality measure  $\frac{1}{\beta_a}u_{a,k}=\frac{1}{a\beta}au_k=\frac{1}{\beta}u_k$  remains the same so it is scaling invariant
- Problem considered solved to optimality if, say,  $\frac{1}{\beta} \|u_k\|_2 \leq 10^{-6}$
- $\bullet$  Often lower accuracy  $10^{-3}$  to  $10^{-4}$  is enough

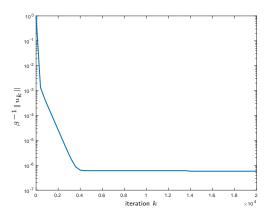
# Example - SVM

- Classification problem from SVM lecture, SVM with
  - polynomial features of degree 2
  - regularization parameter  $\lambda = 0.00001$



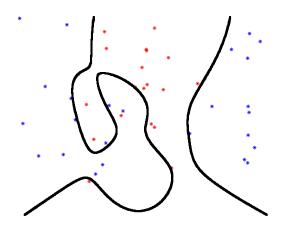
# **Example – Optimality measure**

- $\bullet \ \ \mathsf{Plots} \ \beta^{-1} \|u_k\|_2 = \beta^{-1} \|\gamma_k^{-1}(x_k x_{k+1}) + \nabla f(x_{k+1}) \nabla f(x_k)\|_2$
- Shows  $\beta^{-1}||u_k||_2$  up to 20'000 iterations
- Quite many iterations needed to converge



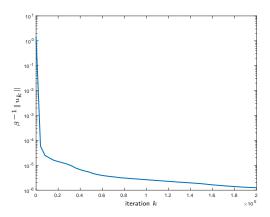
# Example – SVM higher degree polynomial

- Classification problem from SVM lecture, SVM with
  - polynomial features of degree 6
  - regularization parameter  $\lambda = 0.00001$



# Example - Optimality measure

- Plots  $\beta^{-1} \|u_k\|_2 = \beta^{-1} \|\gamma_k^{-1}(x_k x_{k+1}) + \nabla f(x_{k+1}) \nabla f(x_k)\|_2$
- Shows  $\beta^{-1} \|u_k\|_2$  up to 200'000 iterations (10x more than before)
- Many iterations needed for high accuracy



#### Outline

- A fundamental inequality
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# Accelerated proximal gradient method

Consider convex composite problem

$$\min_{x} \min f(x) + g(x)$$

where

- $f: \mathbb{R}^n \to \mathbb{R}$  is  $\beta$ -smooth and convex
- $g: \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$  is closed and convex
- Proximal gradient descent

$$x_{k+1} = \operatorname{prox}_{\gamma g}(x_k - \gamma \nabla f(x_k))$$

achieves O(1/k) convergence rate in function value

• Accelerated proximal gradient method

$$y_k = x_k + \theta_k(x_k - x_{k-1})$$
$$x_{k+1} = \text{prox}_{\gamma g}(y_k - \gamma \nabla f(y_k))$$

(with specific  $\theta_k$ ) achieves faster  $O(1/k^2)$  convergence rate

# Accelerated proximal gradient method - Parameters

Accelerated proximal gradient method

$$y_k = x_k + \theta_k(x_k - x_{k-1})$$
  
$$x_{k+1} = \operatorname{prox}_{\gamma g}(y_k - \gamma \nabla f(y_k))$$

- Step-sizes are restricted  $\gamma \in (0, \frac{1}{\beta}]$
- The  $\theta_k$  parameters can be chosen either as

$$\theta_k = \frac{k-1}{k+2}$$

or  $\theta_k = \frac{t_{k-1}-1}{t_k}$  where

$$t_k = \frac{1 + \sqrt{1 + 4t_{k-1}^2}}{2}$$

these choices are very similar

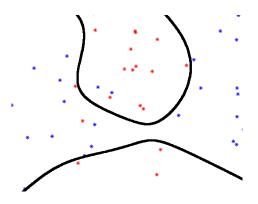
Algorithm behavior in nonconvex setting not well understood

#### Not a descent method

- Descent method means function value is decreasing every iteration
- We know that proximal gradient method is a descent method
- However, accelerated proximal gradient method is not

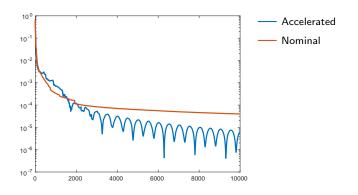
# Accelerated gradient method - Example

- Accelerated vs nominal proximal gradient method
- ullet Problem from SVM lecture, polynomial deg 6 and  $\lambda=0.0215$



# Accelerated gradient method - Example

- Accelerated vs nominal proximal gradient method
- Problem from SVM lecture, polynomial deg 6 and  $\lambda = 0.0215$



#### Outline

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#### Scaled proximal gradient method

Proximal gradient method:

$$x_{k+1} = \underset{y}{\operatorname{argmin}} \left( \underbrace{f(x_k) + \nabla f(x_k)^T (y - x) + \frac{1}{2\gamma_k} \|y - x_k\|_2^2}_{\hat{f}_{x_k}(y)} + g(y) \right)$$

approximates function f(y) around  $x_k$  by  $\hat{f}_{x_k}(y)$ 

- The better the approximation, the faster the convergence
- By scaling: we mean to use an approximation of the form

$$\hat{f}_{x_k}(y) = f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2\gamma_k} ||y - x_k||_H^2$$

where  $H \in \mathbb{R}^{n \times n}$  is a positive definite matrix and  $\|x\|_H^2 = x^T H x$ 

ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



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• Gradient descent on  $\beta$ -smooth quadratic problem

$$\underset{x}{\text{minimize}} \ \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



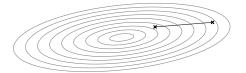
ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



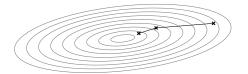
ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



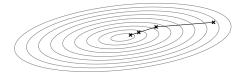
ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



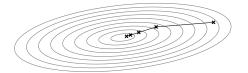
ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



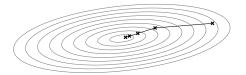
ullet Gradient descent on eta-smooth quadratic problem

$$\underset{x}{\text{minimize}} \quad \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



• Gradient descent on  $\beta$ -smooth quadratic problem

$$\underset{x}{\text{minimize}} \ \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 0.1 & -0.1 \\ -0.1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$



# Smoothness w.r.t. $\|\cdot\|_H$

#### What is $\|\cdot\|_H$ ?

- Requirement:  $H \in \mathbb{R}^{n \times n}$  is symmetric positive definite  $(H \succ 0)$
- ullet The norm  $\|x\|_H^2:=x^THx$ , for H=I, we get  $\|x\|_I^2=\|x\|_2^2$

#### Smoothness

• Function  $f: \mathbb{R}^n \to \mathbb{R}$  is  $\beta$ -smooth if for all  $x, y \in \mathbb{R}^n$ :

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

• We say  $f \ \beta_H$ -smoothness w.r.t. scaled norm  $\|\cdot\|_H$  if

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta_H}{2} ||x - y||_H^2$$
  
$$f(y) \ge f(x) + \nabla f(x)^T (y - x) - \frac{\beta_H}{2} ||x - y||_H^2$$

for all  $x, y \in \mathbb{R}^n$ 

ullet If f is smooth (w.r.t.  $\|\cdot\|_2$ ) it is also smooth w.r.t.  $\|\cdot\|_H$ 

#### Example – A quadratic

- $\bullet$  Let  $f(x) = \frac{1}{2} x^T H x = \frac{1}{2} \|x\|_H^2$  with  $H \succ 0$
- f is 1-smooth w.r.t  $\|\cdot\|_H$  (with equality):

$$\begin{split} f(x) + \nabla f(x)^T (y - x) + \frac{1}{2} \|x - y\|_H^2 \\ &= \frac{1}{2} x^T H x + (Hx)^T (y - x) + \frac{1}{2} \|x - y\|_H^2 \\ &= \frac{1}{2} x^T H x + (Hx)^T (y - x) + \frac{1}{2} (\|x\|_H^2 - 2(Hx)^T y + \|y\|_H^2) \\ &= \frac{1}{2} \|y\|_H^2 = f(y) \end{split}$$

which holds also if adding linear term  $q^T x$  to f

• f is  $\lambda_{\max}(H)$ -smooth (w.r.t.  $\|\cdot\|_2$ ), continue equality:

$$\begin{split} f(y) &= f(x) + \nabla f(x)^T (y-x) + \frac{1}{2} \|x-y\|_H^2 \\ &\leq f(x) + \nabla f(x)^T (y-x) + \frac{\lambda_{\max}(H)}{2} \|x-y\|_2^2 \end{split}$$

much more conservative estimate of function!

# Scaled proximal gradient for quadratics

- Let  $f(x) = \frac{1}{2}x^T H x$  with  $H \succ 0$ , which is 1-smooth w.r.t.  $\|\cdot\|_H$
- Approximation with scaled norm  $\|\cdot\|_H$  and  $\gamma_k = 1$  satisfies  $\forall x_k$ :

$$\hat{f}_{x_k}(y) = f(x_k) + \nabla f(x_k)^T (y - x_k) + \frac{1}{2} ||x_k - y||_H^2 = f(y)$$

since f is 1-smooth w.r.t.  $\|\cdot\|_H$  with equality

An iteration then reduces to solving problem itself:

$$x_{k+1} = \underset{y}{\operatorname{argmin}} (\hat{f}_{x_k}(y) + g(y)) = \underset{y}{\operatorname{argmin}} (f(y) + g(y))$$

Model very accurate, but very expensive iterations

# Scaled proximal gradient method reformulation

• Proximal gradient method with scaled norm  $\|\cdot\|_H$ :

$$x_{k+1} = \underset{y}{\operatorname{argmin}} \left( f(x_k) + \nabla f(x_k)^T (y - x) + \frac{1}{2\gamma_k} \|y - x_k\|_H^2 + g(y) \right)$$
$$= \underset{y}{\operatorname{argmin}} \left( g(y) + \frac{1}{2\gamma_k} \|y - (x_k - \gamma_k H^{-1} \nabla f(x_k))\|_H^2 \right)$$
$$=: \operatorname{prox}_{\gamma_k g}^H (x_k - \gamma_k H^{-1} \nabla f(x_k))$$

where H = I gives nominal method

- Computational difference per iteration:
  - 1. Need to invert  $H^{-1}$  (or solve  $Hd_k = \nabla f(x_k)$ )
  - 2. Need to compute prox with new metric

$$\operatorname{prox}_{\gamma_k g}^H(z) := \underset{x}{\operatorname{argmin}} (g(x) + \frac{1}{2\gamma_k} \|x - z\|_H^2)$$

that may be very costly

#### **Computational cost**

- Assume that H is dense or general sparse
  - $H^{-1}$  dense: cubic complexity (vs maybe quadratic for gradient)
  - $H^{-1}$  sparse: lower than cubic complexity
  - $\operatorname{prox}_{\gamma_k,q}^H$ : difficult optimization problem
- Assume that H is diagonal
  - ullet  $H^{-1}$ : invert diagonal elements linear complexity
  - $\operatorname{prox}_{\gamma_k g}^H$ : often as cheap as nominal prox (e.g., for separable g)
  - this gives individual step-sizes for each coordinate
- Assume that H is block-diagonal with small blocks
  - $H^{-1}$ : invert individual blocks also cheap
  - $\operatorname{prox}_{\gamma_k g}^H$ : often quite cheap (e.g., for block-separable g)
- If H = I, method is nominal method

#### Convergence

- We get similar results as in the nominal H = I case
- We assume  $\beta_H$  smoothness w.r.t.  $\|\cdot\|_H$
- We can replace all  $\|\cdot\|_2$  with  $\|\cdot\|_H$  and  $\nabla f$  with  $H^{-1}\nabla f$ :
  - Nonconvex setting with  $\gamma_k = \frac{1}{\beta_H}$

$$\min_{l \in \{0, \dots, k\}} \|\nabla f(x_l)\|_{H^{-1}}^2 \le \frac{2\beta_H(f(x_0) + g(x_0) - p^*)}{k+1}$$

• Convex setting with  $\gamma_k = \frac{1}{\beta_H}$ 

$$f(x_k) + g(x_k) - p^* \le \frac{\beta_H \|x_0 - x^*\|_H^2}{2(k+1)}$$

• Strongly convex setting with f  $\sigma_H$ -strongly convex w.r.t.  $\|\cdot\|_H$ 

$$||x_{k+1} - x^*||_H \le \max(\beta_H \gamma - 1, 1 - \sigma_H \gamma)||x_k - x^*||_H$$

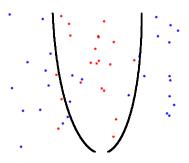
# **Example – Logistic regression**

• Logistic regression with  $\theta = (w, b)$ :

minimize 
$$\sum_{i=1}^{N} \log(1 + e^{w^T \phi(x_i) + b}) - y_i(w^T \phi(x_i) + b) + \frac{\lambda}{2} ||w||_2^2$$

on the following data set (from logistic regression lecture)

- Polynomial features of degree 6, Tikhonov regularization  $\lambda = 0.01$
- Number of decision variables: 28



# **Algorithms**

Compare the following algorithms, all with backtracking:

- 1. Gradient method
- 2. Gradient method with fixed diagonal scaling
- 3. Gradient method with fixed full scaling

#### Fixed scalings

• Logistic regression gradient and Hessian satisfy with L = [X, 1]

$$\nabla f(\theta) = L^T(\sigma(L\theta) - Y) + \lambda I_w \theta \quad \nabla^2 f(\theta) = L^T \sigma'(L\theta) L + \lambda I_w$$

where  $\sigma$  is the (vector-version of) sigmoid, and  $I_w(w,b)=(w,0)$ 

- The sigmoid function  $\sigma$  is 0.25-Lipschitz continuous
- Gradient method with fixed full scaling (3.) uses

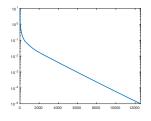
$$H = 0.25L^T L + \lambda I_w$$

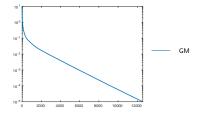
Gradient method with fixed diagonal scaling (2.) uses

$$H = \mathbf{diag}(0.25L^TL + \lambda I_w)$$

# **Example – Numerics**

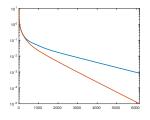
- ullet Logistic regression polynomial features of degree 6,  $\lambda=0.01$
- Standard gradient method with backtracking (GM)

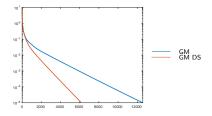




# **Example – Numerics**

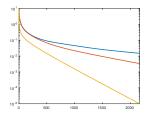
- ullet Logistic regression polynomial features of degree 6,  $\lambda=0.01$
- Gradient method with diagonal scaling (GM DS)

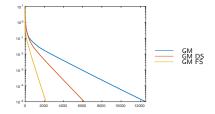




# **Example – Numerics**

- ullet Logistic regression polynomial features of degree 6,  $\lambda=0.01$
- Gradient method with full matrix scaling (GM FS)





#### Comments

- Smaller number of iterations with better scaling
- Performance is roughly (iteration cost)×(number of iterations)
  - We have only compared number of iterations
  - Iteration cost for (GM) and (GM DS) are the same
  - Iteration cost for (GM FS) higher
  - Need to quantify iteration cost to assess which is best
- ullet In general, can be difficult to find H that performs better