Proximal operator and methods

Master 2 Data Science, Univ. Paris Saclay

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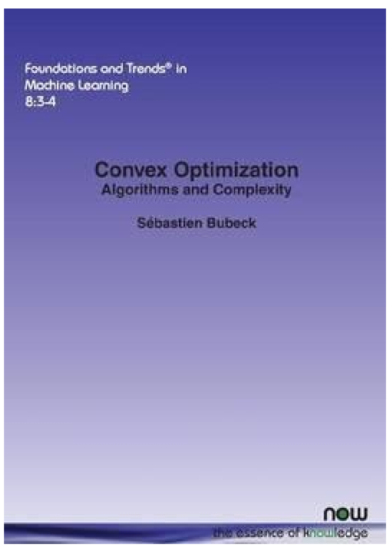
References classes today

Sébastien Bubeck (2015)
Convex Optimization: Algorithms and Complexity



Chapter 1 and Section 5.1

Amir Beck and Marc Teboulle (2009), SIAM J. IMAGING SCIENCES,
A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems.

Optimization Sum of Terms

A Datum Function

$$f_i(w) := \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

$$\begin{aligned} \frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w) &= \frac{1}{n}\sum_{i=1}^{n} \left(\ell\left(h_w(x^i), y^i\right) + \lambda R(w)\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} f_i(w) \end{aligned}$$

Finite Sum Training Problem

$$\min_{w\in\mathbb{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w)$$

The Training Problem

Solving the *training problem*:

$$\min_{w\in\mathbb{R}^d} \frac{1}{n}\sum_{i=1}^n f_i(w)$$

Reference method: Gradient descent

$$\nabla\left(\frac{1}{n}\sum_{i=1}^n f_i(w)\right) = \frac{1}{n}\sum_{i=1}^n \nabla f_i(w)$$

Gradient Descent Algorithm

Set $w^1 = 0$, choose $\alpha > 0$.

for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = w^t - \frac{\alpha}{n}\sum_{i=1}^n \nabla f_i(w^t)$$

Output w^{T+1}

Convergence GD I

Theorem

Let f be convex and L-smooth.

$$f(w^T) - f(w^*) \leq \frac{2L||w^1 - w^*||_2^2}{T-1} = O\left(\frac{1}{T}\right).$$

Where

$$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

$\Rightarrow$ for $\dfrac{f(w^T) - f(w^*)}{||w^1 - w^*||_2^2} \leq \epsilon$ we need $T \geq \dfrac{2L}{\epsilon} = O\left(\dfrac{1}{\epsilon}\right)$

Convergence GD I

Theorem

Let f be convex and L-smooth.

$$f(w^T) - f(w^*) \leq \frac{2L||w^1 - w^*||_2^2}{T-1} = O\left(\frac{1}{T}\right).$$

Where

$$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

Is f always differentiable?

$$\Rightarrow \text{for } \frac{f(w^T) - f(w^*)}{||w^1 - w^*||_2^2} \leq \epsilon \text{ we need } T \geq \frac{2L}{\epsilon} = O\left(\frac{1}{\epsilon}\right)$$

Convergence GD I

Theorem

Let f be convex and L-smooth.

Not true for many problems

$$f(w^T) - f(w^*) \leq \frac{2L||w^1 - w^*||_2^2}{T-1} = O\left(\frac{1}{T}\right).$$

Where

$$w^{t+1} = w^t - \frac{1}{L}\nabla f(w^t)$$

Is f always differentiable?

$$\Rightarrow \text{for } \frac{f(w^T) - f(w^*)}{||w^1 - w^*||_2^2} \leq \epsilon \text{ we need } T \geq \frac{2L}{\epsilon} = O\left(\frac{1}{\epsilon}\right)$$

Change notation: Keep loss and regularizor separate

Loss function

$$L(w) := \frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right)$$

The Training problem

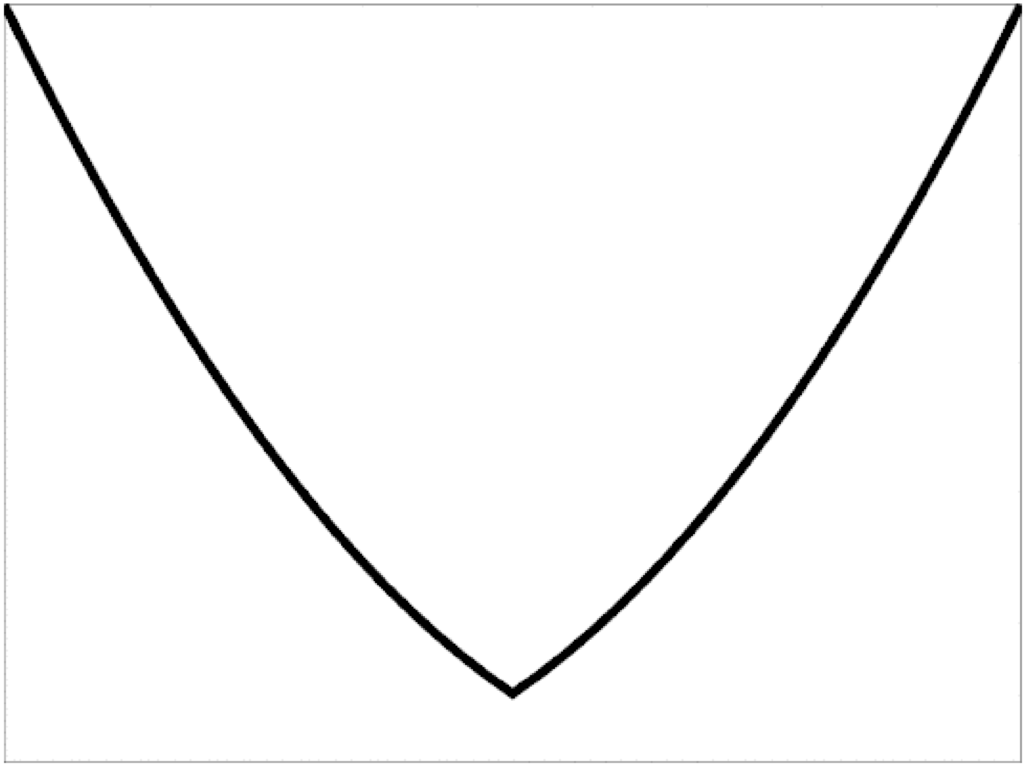
$$\min_w L(w) + \lambda R(w)$$

If L or R is not differentiable $\Rightarrow$ $L+R$ is not differentiable

If L or R is not smooth $\Rightarrow$ $L+R$ is not smooth

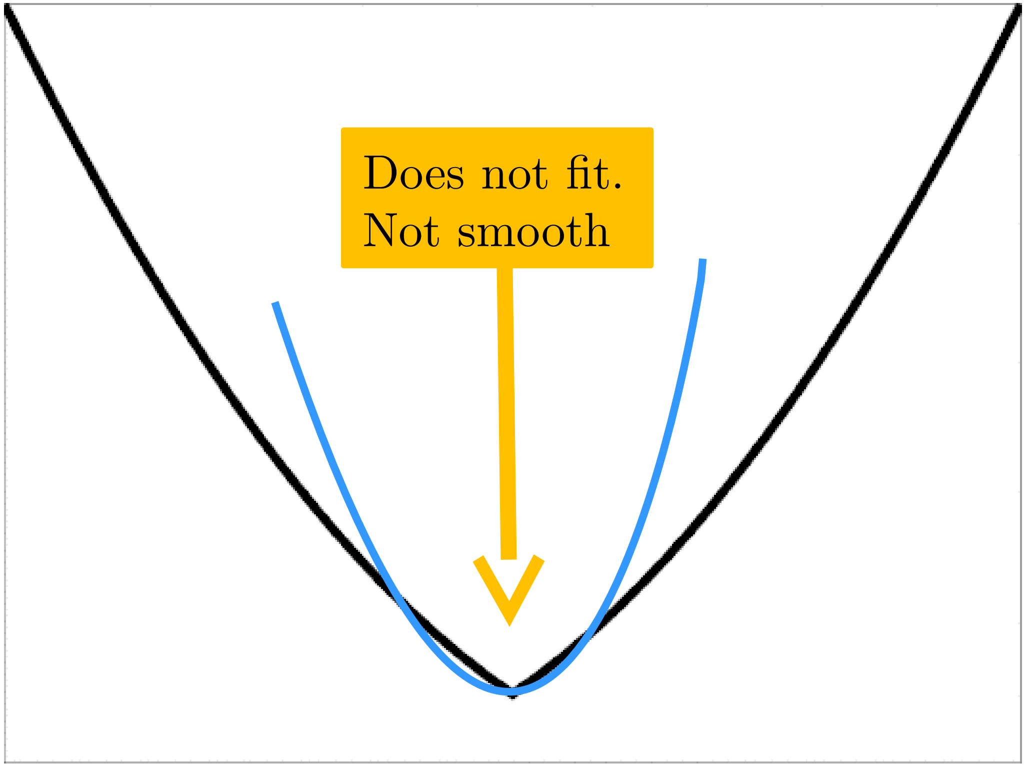
Non-smooth Example

$$L(w) + R(w) = \frac{1}{2}||w||_2^2 + ||w||_1$$



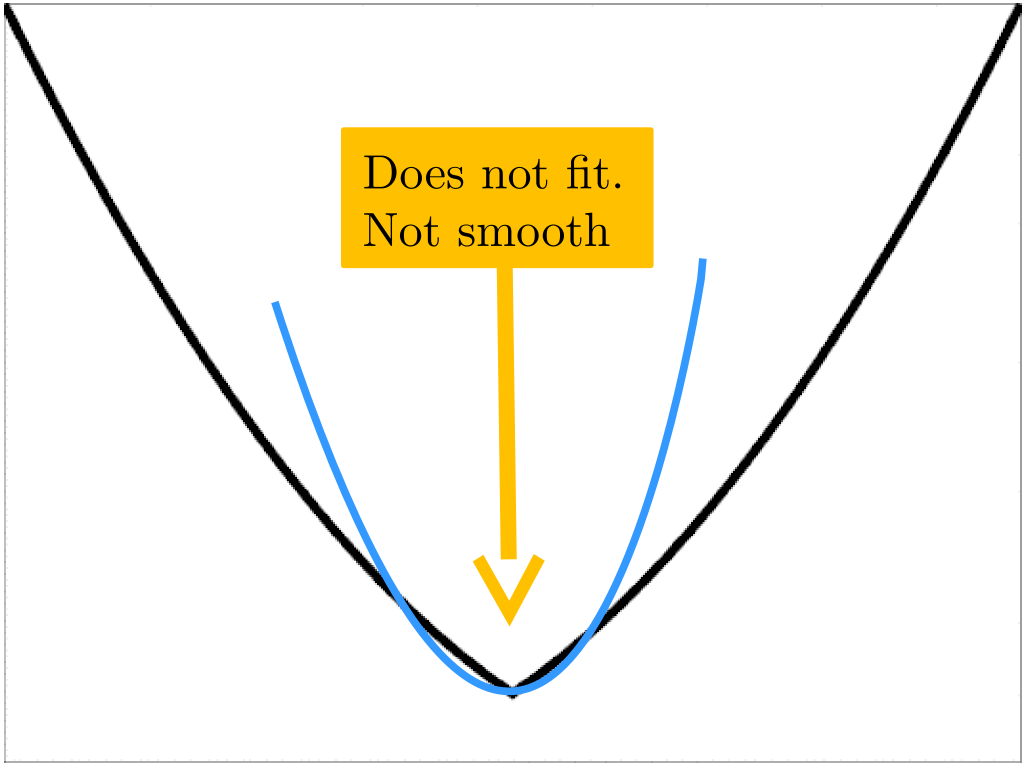
Non-smooth Example

$$L(w) + R(w) = \frac{1}{2}||w||_2^2 + ||w||_1$$



Non-smooth Example

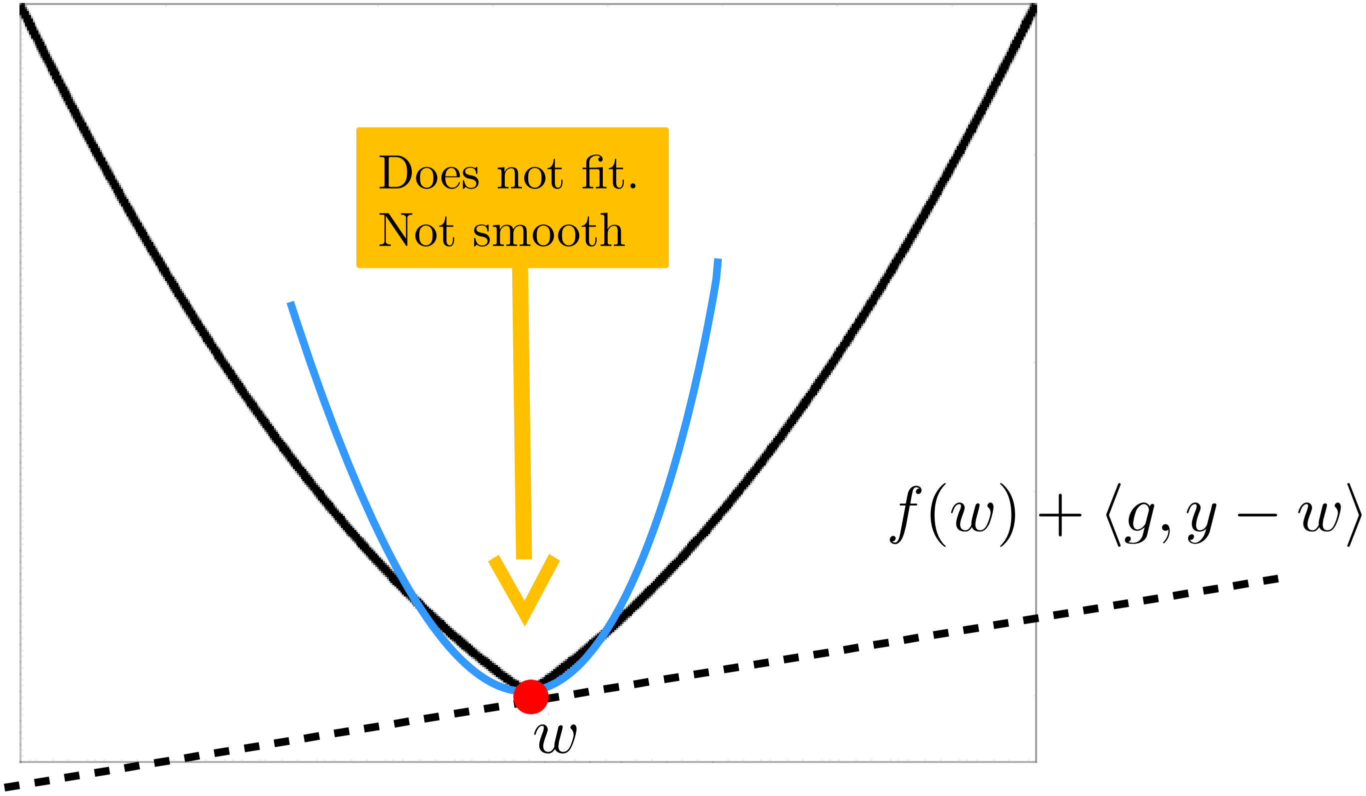
$$L(w) + R(w) = \frac{1}{2}||w||_2^2 + ||w||_1$$



Need more tools

Non-smooth Example

$$L(w) + R(w) = \frac{1}{2}||w||_2^2 + ||w||_1$$



Need more tools

Assumptions for this class

The Training problem

$$\min_{w} L(w) + \lambda R(w)$$

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and "easy to optimize"

What does this mean?

$$\text{prox}_{\gamma R}(y) := \arg\min_{w} \frac{1}{2}||w - y||_2^2 + \gamma R(w)$$

Assume this is easy to solve

Examples

Lasso

$$\min_{w \in \mathbf{R}^d} \frac{1}{2n} \sum_{i=1}^{n} (y^i - \langle w, a^i \rangle)^2 + \lambda ||w||_1$$

Low Rank Matrix Recovery

$$\min_{W \in \mathbf{R}^{d \times d}} \frac{1}{n} \sum_{i=1}^{n} ||AW - Y||_F^2 + \lambda ||W||_*$$

Not smooth, but prox is easy

SVM with soft margin

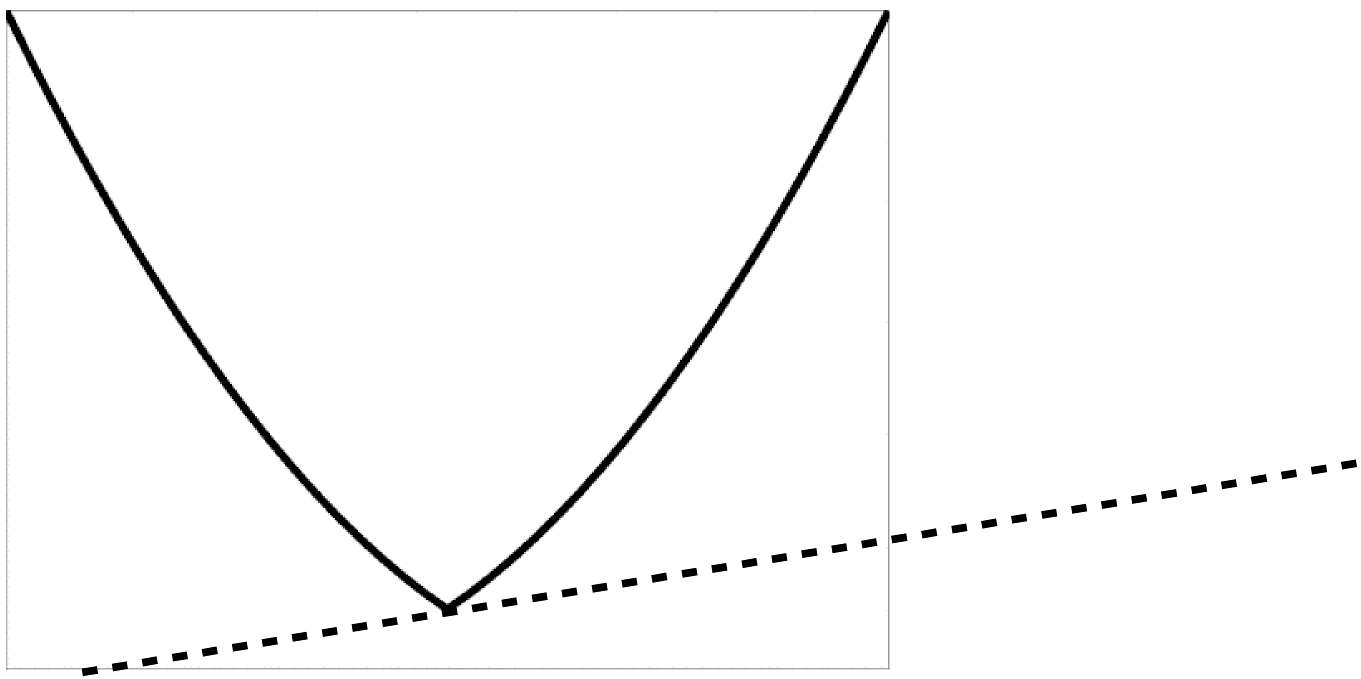
$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y^i \langle w, a^i \rangle\} + \lambda ||w||_2^2$$

Not smooth

Convexity: Subgradient

Let $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ be convex

$$\partial f(w) := \{g \in \mathbb{R}^n \; : \; f(y) \geq f(w) + \langle g, y - w \rangle, \forall y \in \mathrm{dom}(f)\}$$

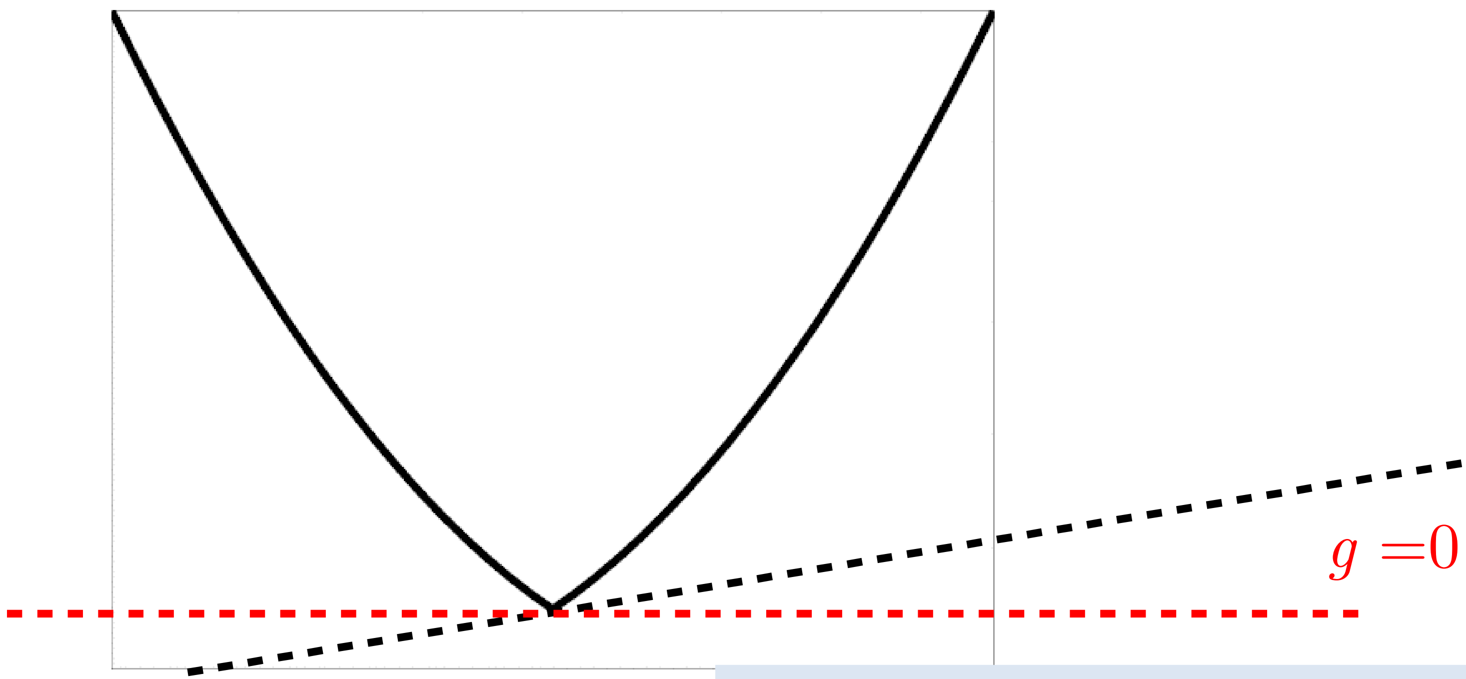


$f(w) + \langle g, y - w \rangle$

Convexity: Subgradient

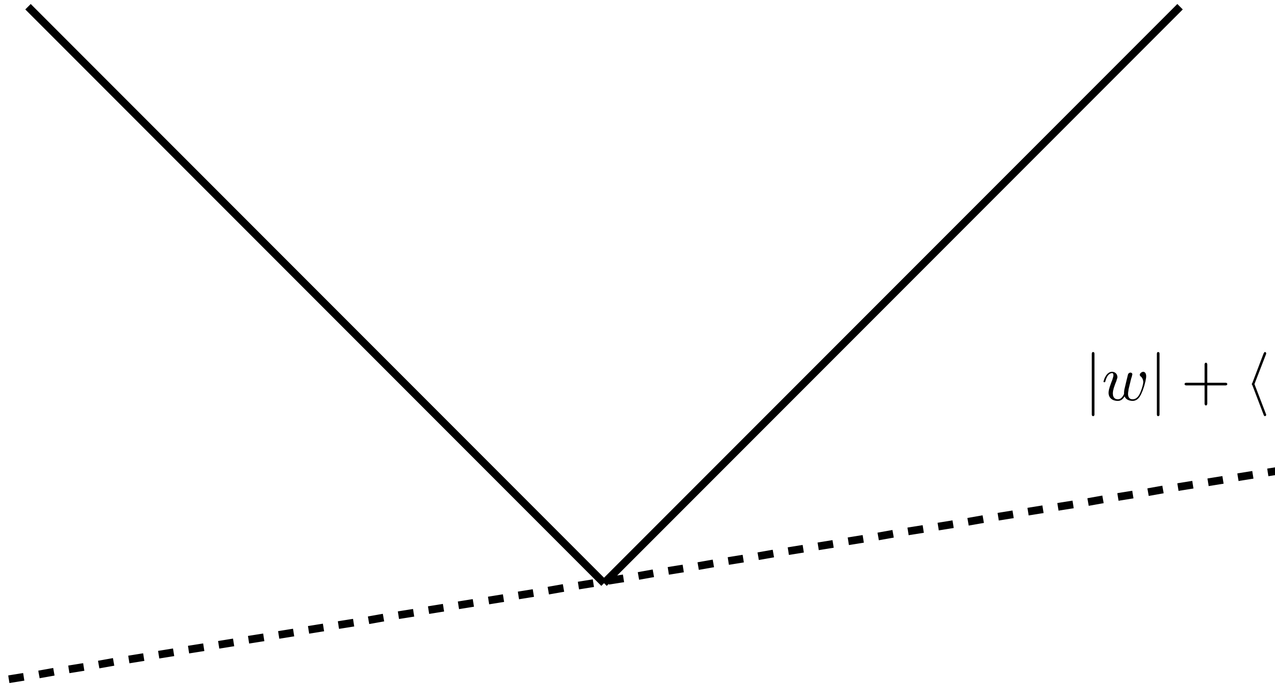
Let $f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ be convex

$$\partial f(w) := \{g \in \mathbb{R}^n \ : \ f(y) \geq f(w) + \langle g, y - w \rangle, \forall y \in \mathrm{dom}(f)\}$$



$$w^* = \arg\min_w f(w) \Leftrightarrow 0 \in \partial f(w^*)$$

Examples: L1 norm



$$|w| + \langle \frac{1}{2}, y - w \rangle$$

$$\partial |w| = \begin{cases} -1 & \text{if } w < 0 \\ [-1,\, 1] & \text{if } w = 0 \\ 1 & \text{if } w > 0 \end{cases}$$

$$\partial ||w||_1 = (\partial |w_1|, \ldots, \partial |w_d|)$$

Optimality conditions

The Training problem

$$w^* = \arg\min_{w \in \mathbf{R}^d} L(w) + \lambda R(w)$$

$$0 \quad \in \quad \partial \left(L(w^*) + \lambda R(w^*) \right) = \nabla L(w^*) + \lambda \partial R(w^*)$$

$$\Downarrow$$

$$-\nabla L(w^*) \in \lambda \partial R(w^*)$$

Working example: Lasso

Lasso

$$\min_{w \in \mathbf{R}^d} \frac{1}{2n} ||Aw - y||_2^2 + \lambda ||w||_1$$

$$A = [a^1, \ldots, a^n]^\top \;\Rightarrow\; \sum_{i=1}^{n} (y^i - \langle w, a^i \rangle)^2 = ||Aw - y||_2^2$$

$$-\nabla L(w^*) \in \partial R(w^*) \quad \Rightarrow \quad -\frac{1}{n} A^\top (Aw^* - y) \in \partial ||w^*||_1$$

Difficult inclusion, do iteratively.

Proximal method I

Using $\mathcal{L}$–smoothness of L :

$$L(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2} ||w - y||^2, \quad \forall w, y \in \mathbb{R}^d$$

The w that minimizes the upper bound gives gradient descent

$$w = y - \frac{1}{\mathcal{L}} \nabla L(y)$$

Proximal method I

Using $\mathcal{L}$–smoothness of L :

$$L(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2} ||w - y||^2, \quad \forall w, y \in \mathbb{R}^d$$

The w that minimizes the upper bound gives gradient descent

$$w = y - \frac{1}{\mathcal{L}} \nabla L(y)$$

But what about *R(w)*? Adding on $+\lambda R(w)$ to upper bound:

Proximal method I

Using $\mathcal{L}$–smoothness of L :

$$L(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2, \quad \forall w, y \in \mathbb{R}^d$$

The w that minimizes the upper bound gives gradient descent

$$w = y - \frac{1}{\mathcal{L}} \nabla L(y)$$

But what about $R(w)$? Adding on $+\lambda R(w)$ to upper bound:

$$\boxed{L(w) + \lambda R(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2 + \lambda R(w)}$$

Proximal method I

Using $\mathcal{L}$–smoothness of L :

$$L(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2, \quad \forall w, y \in \mathbb{R}^d$$

The w that minimizes the upper bound gives gradient descent

$$w = y - \frac{1}{\mathcal{L}} \nabla L(y)$$

But what about *R(w)*? Adding on $+\lambda R(w)$ to upper bound:

$$\boxed{L(w) + \lambda R(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2 + \lambda R(w)}$$

Can we minimize the right-hand side?

Proximal method II

Minimizing the right-hand side of

$$L(w) + \lambda R(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2} ||w - y||^2 + \lambda R(w)$$

$$\begin{aligned}
&\arg\min_w L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2} ||w - y||^2 + \lambda R(w) \\
&\qquad = \arg\min_w \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2} ||w - y||^2 + \lambda R(w) \\
&\qquad = \arg\min_w \frac{1}{2} ||w - (y - \frac{1}{\mathcal{L}} \nabla L(y))||^2 + \frac{\lambda}{\mathcal{L}} R(w) \\
&\qquad =: \mathrm{prox}_{\frac{\lambda}{\mathcal{L}} R}(y - \frac{1}{\mathcal{L}} \nabla L(y)))
\end{aligned}$$

What is this prox operator?

$$\mathrm{prox}_{\frac{\lambda}{\mathcal{L}} R}(v) := \arg\min_w \frac{1}{2} ||w - v||_2^2 + \frac{\lambda}{\mathcal{L}} R(w)$$

Gradient Descent using proximal map

$$\mathrm{prox}_{\gamma R}(y) := \arg\min_{w} \frac{1}{2}||w-y||_2^2 + \gamma R(w)$$

EXE: Let

$$f(y) + \langle \nabla f(y), w-y\rangle =: \ell(y,w)$$

Show that

$$\mathrm{prox}_{\gamma \ell(y,\cdot)}(y) = y - \gamma \nabla f(y)$$

A gradient step is also a proximal step

Proximal Operator I

Let $f(x)$ be a convex function. The proximal operator is

$$\text{prox}_f(v) := \arg\min_w \frac{1}{2}||w - v||_2^2 + f(w)$$

Let $w_v = \text{prox}_f(v)$. Using optimality conditions

$$0 \in \partial \left(\tfrac{1}{2}||w_v - v||_2^2 + f(w)\right) = w_v - v + \partial f(w_v)$$

Rearranging

$$\text{prox}_f(v) = w_v \in v - \partial f(w_v)$$

EXE: Is this Proximal operator well defined? Is it even a function?

Proximal Operator II: Optimality conditions

The Training problem

$$\min_{w} L(w) + \lambda R(w)$$

$$-\nabla L(w^*) \in \lambda \partial R(w^*)$$

$$w^* + \gamma \nabla L(w^*) \in w^* - (\lambda\gamma)\partial R(w^*)$$

$$w^* \in (w^* - \gamma \nabla L(w^*)) - (\lambda\gamma)\partial R(w^*)$$

$$\downarrow$$

$$\mathrm{prox}_f(v) = w_v \in v - \partial f(w_v)$$

$$w^* = \mathrm{prox}_{\lambda\gamma R}(w^* - \gamma \nabla L(w^*))$$

Optimal is a fixed point.

Proximal Operator III: Properties

$$\mathrm{prox}_f(v) := \arg\min_w \frac{1}{2}||w - v||_2^2 + f(w)$$

Exe:

1) If $f(w) = \sum_{i=1}^{d} f_i(w_i)$ then

$$\mathrm{prox}_f(v) = (\mathrm{prox}_{f_1}(v_1), \ldots, \mathrm{prox}_{f_d}(v_d))$$

2) If $f(w) = I_C(w) := \begin{cases} 0 & \text{if } w \in C \\ \infty & \text{if } w \notin C \end{cases}$ where C is closed and convex then $\mathrm{prox}_f(v) = \mathrm{proj}_C(v)$

3) If $f(w) = \langle b, w\rangle + c$ then $\mathrm{prox}_f(v) = v - b$

4) If $f(w) = \frac{\lambda}{2} w^\top A w + \langle b, w\rangle$ where $A \succeq 0,\ A = A^\top, \lambda \geq 0$ then

$$\mathrm{prox}_f(v) = (I + \lambda A)^{-1}(v - b)$$

Proximal Operator IV: Soft thresholding

$$\text{prox}_{\lambda||w||_1}(v) := \arg\min_w \frac{1}{2}||w-v||_2^2 + \lambda||w||_1$$

Exe:

1) Let $\alpha \in \mathbf{R}$. If $\alpha^* = \arg\min_{\alpha} \frac{1}{2}(\alpha - v)^2 + \lambda|\alpha|$ then

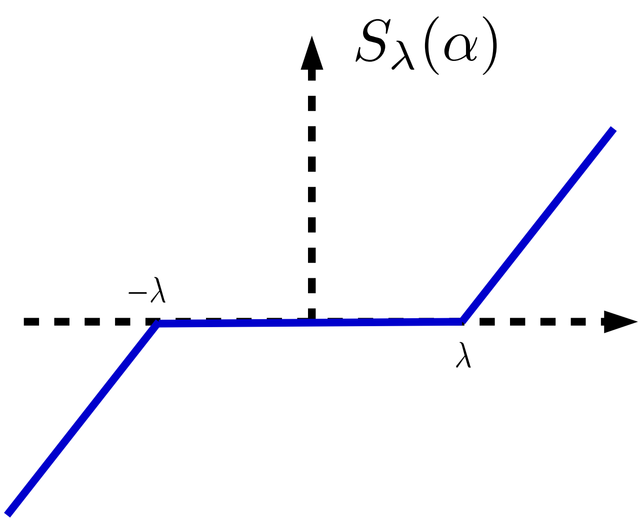
$$\alpha^* \in v - \lambda\partial|\alpha^*| \qquad (I)$$

2) If $\lambda < v$ show (I) gives $\alpha^* = v - \lambda$

3) If $v < -\lambda$ show (I) gives $\alpha^* = v + \lambda$

4) Show that

$$\text{prox}_{\lambda|\alpha|}(v) = \begin{cases} v - \lambda & \text{if } \lambda < v \\ 0 & \text{if } -\lambda \leq v \leq \lambda \\ v + \lambda & \text{if } v < -\lambda. \end{cases}$$



Proximal Operator V: Singular value thresholding

$$S_\lambda(v) := \arg\min_w \frac{1}{2}||w - v||_2^2 + \lambda||w||_1$$

Similarily, the prox of the nuclear norm for matrices:

$$U\mathrm{diag}(S_\lambda(\mathrm{diag}(\sigma(A))))V^\top := \arg\min_{W \in \mathbf{R}^{d\times d}} \frac{1}{2}||W - A||_F^2 + \lambda||W||_*$$

where $A = U\mathrm{diag}(\sigma(A))V^\top$ is a SVD decomposition.

Proximal method V

Minimizing the right-hand side of

$$L(w) + \lambda R(w) \leq L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2 + \lambda R(w)$$

$$\begin{aligned}
&\arg\min_w L(y) + \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2 + \lambda R(w) \\
&\quad = \arg\min_w \langle \nabla L(y), w - y \rangle + \frac{\mathcal{L}}{2}||w - y||^2 + \lambda R(w) \\
&\quad = \arg\min_w \frac{1}{2}||w - (y - \frac{1}{\mathcal{L}}\nabla L(y)||^2 + \frac{\lambda}{\mathcal{L}} R(w)
\end{aligned}$$

$$= \mathrm{prox}_{\frac{\lambda}{\mathcal{L}}R}\left(y - \frac{1}{\mathcal{L}}\nabla L(w)\right)$$

Make iterative method based on this upper bound minimization

The Proximal Gradient Method

Solving the *training problem*:

$$\min_{w} L(w) + \lambda R(w)$$

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and prox friendly

Proximal Gradient Descent

Set $w^1 = 0$.
for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = \mathrm{prox}_{\lambda R/\mathcal{L}} \left(w^t - \frac{1}{\mathcal{L}} \nabla L(w^t) \right)$$

Output w^{T+1}

Iterative Soft Thresholding Algorithm (ISTA)

Lasso

$$\min_{w \in \mathbf{R}^d} \frac{1}{2n} ||Aw - y||_2^2 + \lambda ||w||_1$$

$$A = [a^1, \ldots, a^n]^\top \Rightarrow \sum_{i=1}^{n} (y^i - \langle w, a^i \rangle)^2 = ||Aw - y||_2^2$$

ISTA:

$$w^{t+1} = \text{prox}_{\lambda ||w||_1 / \mathcal{L}} \left(w^t - \frac{1}{n\mathcal{L}} A^\top (Aw^t - y) \right)$$

$$\mathcal{L} = \frac{\sigma_{\max}(A)^2}{n}$$

$$= S_{\lambda/\mathcal{L}} \left(w^t - \frac{1}{\sigma_{\max}(A)^2} A^\top (Aw^t - y) \right)$$

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Amir Beck and Marc Teboulle (2009), SIAM J. IMAGING SCIENCES,
A Fast Iterative Shrinkage-Thresholding Algorithm
for Linear Inverse Problems.

Convergence of Prox-GD

Theorem (Beck Teboulle 2009)

Let $f(w) = L(w) + \lambda R(w)$ where

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and prox friendly

Then

$$f(w^T) - f(w^*) \leq \frac{L||w^1 - w^*||_2^2}{2T} = O\left(\frac{1}{T}\right).$$

where

$$w^{t+1} = w^{t+1} = \text{prox}_{\lambda R/\mathcal{L}}\left(w^t - \frac{1}{\mathcal{L}}\nabla L(w^t)\right)$$

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Convergence of Prox-GD

Theorem (Beck Teboulle 2009)

Let $f(w) = L(w) + \lambda R(w)$ where

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and prox friendly

Can we do better?

Then

$$f(w^T) - f(w^*) \leq \frac{L||w^1 - w^*||_2^2}{2T} = O\left(\frac{1}{T}\right).$$

where

$$w^{t+1} = w^{t+1} = \mathrm{prox}_{\lambda R/\mathcal{L}}\left(w^t - \frac{1}{\mathcal{L}}\nabla L(w^t)\right)$$

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Amir Beck and Marc Teboulle (2009), SIAM J. IMAGING SCIENCES,
A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems.

The FISTA Method

Solving the *training problem*:

$$\min_{w} L(w) + \lambda R(w)$$

The FISTA Algorithm

Set $w^1 = 0 = z^1, \beta^1 = 1$

for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = \text{prox}_{\lambda R/\mathcal{L}}\left(z^t - \frac{1}{\mathcal{L}}\nabla L(z^t)\right)$$

$$\beta^{t+1} = \frac{1 + \sqrt{1 + 4(\beta^t)^2}}{2}$$

$$z^{t+1} = w^{t+1} + \frac{\beta^t - 1}{\beta^{t+1}}(w^{t+1} - w^t)$$

Output w^{T+1}

The FISTA Method

Solving the *training problem*:

$$\min_w L(w) + \lambda R(w)$$

The FISTA Algorithm

Set $w^1 = 0 = z^1, \beta^1 = 1$

for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = \operatorname{prox}_{\lambda R/\mathcal{L}}\left(z^t - \frac{1}{\mathcal{L}}\nabla L(z^t)\right)$$

$$\beta^{t+1} = \frac{1 + \sqrt{1 + 4(\beta^t)^2}}{2}$$

$$z^{t+1} = w^{t+1} + \frac{\beta^t - 1}{\beta^{t+1}}(w^{t+1} - w^t)$$

Output w^{T+1}

Weird, but it works

Convergence of FISTA

Theorem (Beck Teboulle 2009)

Let $f(w) = L(w) + \lambda R(w)$ where

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and prox friendly

Then

$$f(w^T) - f(w^*) \leq \frac{2L||w^1 - w^*||_2^2}{(T+1)^2} = O\left(\frac{1}{T^2}\right).$$

Where w^t are given by the FISTA algorithm

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Convergence of FISTA

Theorem (Beck Teboulle 2009)

Let $f(w) = L(w) + \lambda R(w)$ where

$L(w)$ is differentiable, $\mathcal{L}$–smooth and convex

$R(w)$ is convex and prox friendly

Is this as good as it gets?

Then

$$f(w^T) - f(w^*) \leq \frac{2L||w^1 - w^*||_2^2}{(T+1)^2} = O\left(\frac{1}{T^2}\right).$$

Where w^t are given by the FISTA algorithm

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Lab Session 01.10

Bring your laptop!

Lab Session 01.10

Bring your laptop!

Introduction to Stochastic Gradient Descent

Optimization Sum of Terms

A Datum Function

$$f_i(w) := \ell\left(h_w(x^i), y^i\right) + \lambda R(w)$$

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} \ell\left(h_w(x^i), y^i\right) + \lambda R(w) &= \frac{1}{n}\sum_{i=1}^{n} \left(\ell\left(h_w(x^i), y^i\right) + \lambda R(w)\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} f_i(w)\end{aligned}$$

Finite Sum Training Problem

$$\min_{w \in \mathbf{R}^d} \frac{1}{n}\sum_{i=1}^{n} f_i(w) =: f(w)$$

The Training Problem

Solving the *training problem*: $$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Reference method: Gradient descent

$$\nabla \left(\frac{1}{n} \sum_{i=1}^{n} f_i(w) \right) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w)$$

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.

for $t = 1, 2, 3, \ldots, T$

$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$

Output w^{T+1}

The Training Problem

Solving the *training problem*:

$$\min_{w \in \mathbf{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(w)$$

Problem with Gradient Descent:
Each iteration requires computing a gradient $\nabla f_i(w)$ for each data point. One gradient for each cat on the internet!

Gradient Descent Algorithm

Set $w^0 = 0$, choose $\alpha > 0$.
for $t = 1, 2, 3, \ldots, T$
$$w^{t+1} = w^t - \frac{\alpha}{n} \sum_{i=1}^{n} \nabla f_i(w^t)$$
Output w^{T+1}

Stochastic Gradient Descent

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Use $\nabla f_j(w) \approx \nabla f(w)$

Stochastic Gradient Descent

Stochastic Gradient Descent Algorithm

Set $w^0 = 0,$ choose $\alpha > 0.$

for $t = 1, 2, 3, \ldots, T$

Sample $j \in \{1, \ldots, n\}$

$w^{t+1} = w^t - \alpha \nabla f_j(w^t)$

Output w^{T+1}