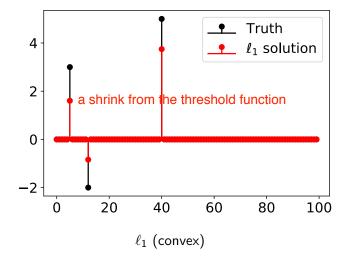
Algorithms for non-convex optimization in ML

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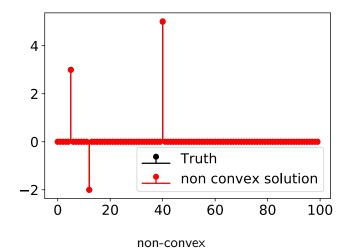


Master 2 Data Science, Univ. Paris Saclay Optimisation for Data Science

Why non-convexity matters?



Why non-convexity matters?



Non-convexity and machine learning

- Sparsity is a way to do feature selection while learning
- ℓ_1 regularization is just a convex surrogate of the ℓ_0 pseudo-norm which is the true quantification of sparsity.
- General non-convex optimization is (too) hard
- but for machine learning, e.g., F(x) = f(x) + g(x) there is hope!
- We'll focus on non-convex regularizations

Motivation

Use a non-convex separable penalty $g(x) = \sum_i g_i(x^{(i)}) \approx ||x||_0$:

$$\hat{x} = \operatorname*{arg\,min}_{x \in \mathbb{R}^n} \quad \left(\quad \underbrace{f(x)}_{\text{data fit}} \quad + \underbrace{\sum_{i=1}^n g_i(x^{(i)})}_{\text{regularization}} \right)$$

also in coordinate descend

Use a non-convex separable penalty $g(x) = \sum_i g_i(x^{(i)}) \approx ||x||_0$:

$$\hat{x} = \underset{x \in \mathbb{R}^n}{\min} \quad \left(\quad \underbrace{f(x)}_{\text{data fit}} \quad + \underbrace{\sum_{i=1}^n g_i(x^{(i)})}_{\text{regularization}} \right)$$

 Adaptive-Lasso Zou (2006) / ℓ₁ reweighted Candès et al. (2008)

$$g_i(t) = \lambda |t|^q$$
 with $0 < q < 1$

Use a non-convex separable penalty $g(x) = \sum_i g_i(x^{(i)}) \approx ||x||_0$:

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• ℓ_1 reweighted Candès *et al.* (2008)

$$g_i(t) = \lambda \log(1 + |t|/\gamma)$$

Use a non-convex separable penalty $g(x) = \sum_i g_i(x^{(i)}) \approx ||x||_0$:

$$\hat{x} = \underset{x \in \mathbb{R}^n}{\min} \quad \left(\quad \underbrace{f(x)}_{\text{data fit}} \quad + \underbrace{\sum_{i=1}^n g_i(x^{(i)})}_{\text{regularization}} \right)$$

• MCP (minimax concave penalty) Zhang (2010) for $\lambda > 0$ and $\gamma > 1$

$$g_i(t) = egin{cases} \lambda |t| - rac{t^2}{2\gamma}, & ext{if } |t| \leq \gamma \lambda \ rac{1}{2} \gamma \lambda^2, & ext{if } |t| > \gamma \lambda \end{cases}$$

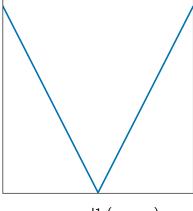
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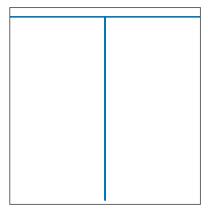
• SCAD (Smoothly Clipped Absolute Deviation) Fan et Li (2001) for $\lambda > 0$ and $\gamma > 2$

$$g_i(t) = egin{cases} \lambda |t|, & ext{if } |t| \leq \lambda \ rac{\gamma \lambda |t| - (t^2 + \lambda^2)/2}{\gamma - 1}, & ext{if } \lambda < |t| \leq \gamma \lambda \ rac{\lambda^2 (\gamma^2 - 1)}{2(\gamma - 1)}, & ext{if } |t| > \gamma \lambda \end{cases}$$

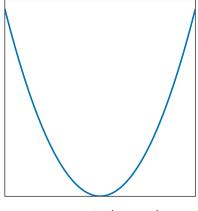
Remark: theoretically and algorithmically difficult (stopping criteria, local minima, etc.)



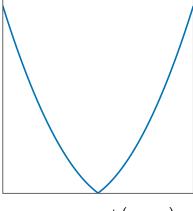
I1 (convex)



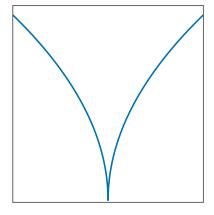
10 (non-convex)



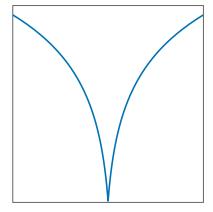
I2 (convex)



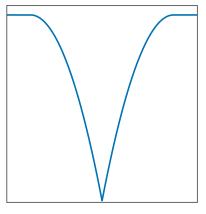
enet (convex)



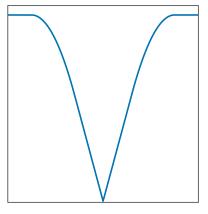
sqrt (non-convex)



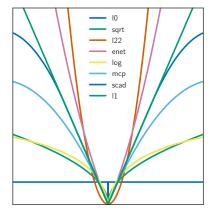
log (non-convex)



mcp (non-convex)



scad (non-convex)



CD for composite separable problem

We consider:

$$F(x) = f(x) + \sum_{i=1}^{n} g_i(x^{(i)})$$
,

with

- f convex, differentiable
- $g(x) = \sum_{i} g_{i}(x^{(i)})$ separable
- each g_i convex or non-convex

Proximal coordinate descent

Parameters: $\gamma_1, \ldots, \gamma_n > 0$

Algorithm:

Choose
$$i_{k+1} \in \{1, ..., n\}$$

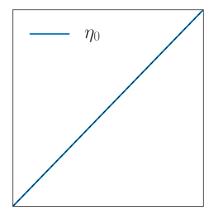
$$\begin{cases} x_{k+1}^{(i)} = \eta_{\gamma_i g_i} \left(x_k^{(i)} - \gamma_i \nabla_i f(x_k) \right) & \text{if } i = i_{k+1} \\ x_{k+1}^{(i)} = x_k^{(i)} & \text{if } i \neq i_{k+1} \end{cases}$$

$$\eta_{\gamma_i g_i}(z) = \operatorname{arg\,min}_{x \in \mathbb{R}} g_i(x) + \frac{1}{2\gamma_i} (x-z)^2$$
 (Prox. operator)

Remark: In non-convex case no guarantee to find a global minimum.

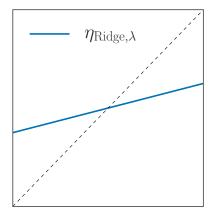
Regularization (1D): No $g_i(z) = 0$

$$\eta_0(z)=z$$



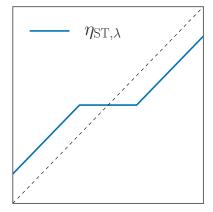
Regularization (1D): Ridge $g_i(z) = z^2$

$$\eta_{\mathrm{Ridge},\lambda}(z) = \frac{z}{1+\lambda}$$



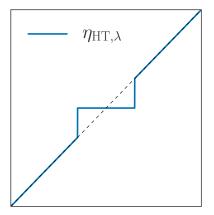
Regularization (1D): Lasso $g_i(z) = |z|$

$$\eta_{\text{ST},\lambda}(z) = \text{sign}(z)(|z| - \lambda)_{+}$$



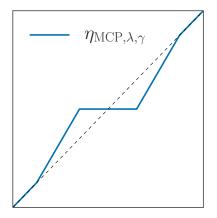
Regularization (1D): ℓ_0 $g_i(z) = \mathbf{1}_{z eq 0}$

$$\eta_{\mathrm{HT},\lambda^2/2}(z)=z\mathbf{1}_{|z|\geq\lambda}$$



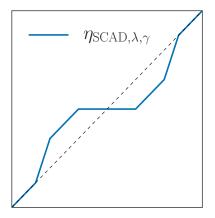
Regularization (1D): MCP

$$\eta_{\mathrm{MCP},\lambda,\gamma}(z) = egin{cases} \mathrm{sign}(z)(|z|-\lambda)_+/(1-1/\gamma) & \mathrm{if}\ |z| \leq \gamma\lambda \ z & \mathrm{if}\ |z| > \gamma\lambda \end{cases}$$



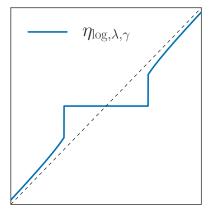
Regularization (1D): SCAD

$$\eta_{\mathrm{SCAD},\lambda,\gamma}(z) = egin{cases} \mathrm{sign}(z)(|z|-\lambda)_+/(1-1/\gamma) & \text{if } |z| \leq 2\lambda \ ([\gamma-1)z-\mathrm{sign}(z)\gamma\lambda]/(\gamma-2) & \text{if } 2\lambda \leq |z| \leq \gamma\lambda \ z & \text{if } |z| > \gamma\lambda \end{cases}$$



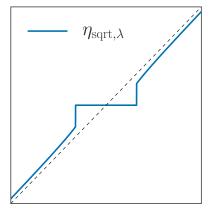
Regularization (1D): $\log g_i(z) = \log(\varepsilon + |z|)$

$$\eta_{\log,\lambda}(z) = \dots$$



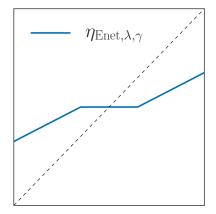
Regularization (1D): sqrt
$$g_i(z) = \sqrt{|z|}$$

$$\eta_{\operatorname{sqrt},\lambda}(z) = \dots$$

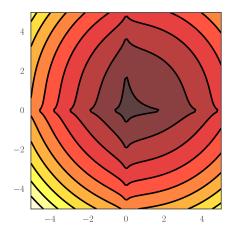


Regularization (1D): Enet $g_i(z) = \rho |z| + (1 - \rho)z^2$

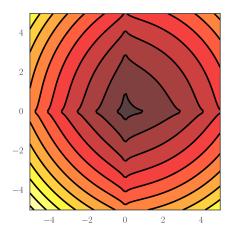
$$\eta_{Enet,\lambda,\gamma}(z) = \dots$$



Level lines for log



Level lines for sqrt



Prox. CD with squared loss

Let $f(x) = \frac{1}{2}||y - Ax||^2$, where $y \in \mathbb{R}^m$, $A \in \mathbb{R}^{m \times n}$ is the design matrix with columns A_1, \ldots, A_n (one per feature)

Consider minimizing over $x^{(i)}$, with all $x^{(j)}$, $j \neq i$ fixed.

We obtain:

$$x^{(i)} \leftarrow \eta_{\frac{1}{\|A_i\|^2}g_i} \left(x^{(i)} + \frac{A_i^\top r}{\|A_i\|^2} \right)$$

where r = y - Ax is the current residual.

Repeat these updates by cycling or random pass over coordinates.

 \rightarrow notebook

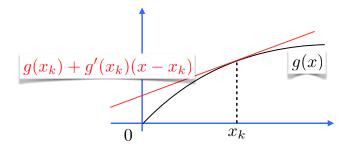
Motivation

Many names for the same idea:

- Adaptive-Lasso Zou (2006)
- ℓ_1 reweighted Candès et al. (2008)
- DC-programming (for *Difference of Convex Programming*) Gasso et al. (2008)

Intuition for adaptive-Lasso & Majorization-Minimization

A non-convex concave function can be upper bounded by its tangent:



The idea of Majorization-Minimization (MM) is to minimize convex majorant functions iteratively.

Adaptive Lasso (for q = 1/2)

Example: take g_j concave e.g. $g_j(t) = \lambda |t|^q$ with q = 1/2

Require: X, \mathbf{y} , number of iterations K, regularization λ

- 1: Initialization: $\hat{w} \leftarrow (1, \dots, 1)^{\top}$
- 2: **for** k = 1, ..., K **do**

3:
$$\hat{\boldsymbol{\theta}} \leftarrow \operatorname*{arg\,min}_{\boldsymbol{\theta}} \left(\frac{\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2}{2} + \lambda \sum_{j=1}^p \hat{w}_j |\theta_j| \right)$$

- 4: $\hat{w}_j \leftarrow g_j'(\hat{\theta}_j), \forall j \in \llbracket 1, p \rrbracket$
- 5: end for

变量代换: 使用lasso funciton

6: return $\hat{\theta}$

Remark: in practice no need to do many iterations (5 iterations)

Remark: use a Lasso solver to update $\hat{\boldsymbol{\theta}}$

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