Non-negative Least Squares

PGD, accelerated PGD and with restart

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Overview

Non-negative Least Squares

Non-**N**egative **L**east **S**quares (NNLS) : given $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$, find $\mathbf{x} \in \mathbb{R}^n_{+}$ by solving

$$\mathbf{x}_{\text{NNLS}} := \arg\min_{\mathbf{x} \geq 0} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$$

A constrained optimization problem: $\mathbf{x}$ has to be non-negative.

- $\mathbf{x}$ is the *coefficient*
- $\mathbf{x}_{\text{NNLS}}$ tells the contributions of each columns $\mathbf{a}_i$ towards $\mathbf{b}$
- $\mathbf{x}_{\text{LS}}$ is less interpretable as coefficient $\mathbf{x}_{\text{LS}}$ can has mixed signs, leading to mutual elimination

Equivalent constrained QP formulation of NNLS

Expand the function $\frac{1}{2}\|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^2$:

$$\begin{aligned}
f(\mathbf{x}) &= \frac{1}{2}(\mathbf{A}\mathbf{x}-\mathbf{b})^\top(\mathbf{A}\mathbf{x}-\mathbf{b}) \\
&= \frac{1}{2}\Big(\mathbf{x}^\top\mathbf{A}^\top\mathbf{A}\mathbf{x}-\mathbf{x}^\top\mathbf{A}^\top\mathbf{b}-\mathbf{b}^\top\mathbf{A}\mathbf{x}+\mathbf{b}^\top\mathbf{b}\Big) \\
&= \frac{1}{2}\Big(\mathbf{x}^\top\mathbf{A}^\top\mathbf{A}\mathbf{x}-2\mathbf{b}^\top\mathbf{A}\mathbf{x}+\|\mathbf{b}\|_2^2\Big) \\
&= \frac{1}{2}\mathbf{x}^\top\mathbf{A}^\top\mathbf{A}\mathbf{x}-\mathbf{b}^\top\mathbf{A}\mathbf{x}+\frac{1}{2}\|\mathbf{b}\|_2^2.
\end{aligned}$$

Let $\mathbf{Q}=\mathbf{A}^\top\mathbf{A}$, $\mathbf{p}=(\mathbf{b}^\top\mathbf{A})^\top=-\mathbf{A}^\top\mathbf{b}$ and $c=\frac{1}{2}\|\mathbf{b}\|_2^2$, NNLS becomes a constrained quadratic programming (QP) problem

$$\min_{\mathbf{x}\geq 0}\frac{1}{2}\mathbf{x}^\top\mathbf{Q}\mathbf{x}-\mathbf{p}^\top\mathbf{x}+c.$$

In the following, we ignore the constant c

NNLS(NNQP) is a convex problem

$$\min_{\mathbf{x}\in\mathbb{R}^n_{+}} \frac{1}{2}\mathbf{x}^\top\mathbf{Q}\mathbf{x} - \mathbf{p}^\top\mathbf{x},\ \mathbf{Q} = \mathbf{A}^\top\mathbf{A},\ \mathbf{p} = \mathbf{A}^\top\mathbf{b}.$$

- matrix $\mathbf{Q} = \mathbf{A}^\top\mathbf{A}$ is always positive-semidefinite and symmetric
- If $\mathbf{A}$ is full rank then $\mathbf{Q}$ is positive-definite
- NNLS(NNQP) is a convex optimization problem.
  - the function convex : it is quadratic
  - the constraint set is convex : it is the positive orthant

Solving NNLS by pseudo inverse and projection

The simplest (but wrong) way to solve NNLS is to modify the solution obtained from the corresponding ordinary least squares: if $\mathbf{A}^\top\mathbf{A}$ is invertible, set gradient equation $\nabla f(\mathbf{x}) = \mathbf{A}^\top\mathbf{A}\mathbf{x} - \mathbf{A}^\top\mathbf{b}$ zero we get

$$\mathbf{x}_{\mathsf{LS}} = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top\mathbf{b}$$

Now we have a two-step method to solve the NNLS

1. $\mathbf{y} = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top\mathbf{b}$ (solution of ordinary least squares)
2. $\mathbf{x} = \mathcal{P}_{\mathbb{R}^n_+}(\mathbf{y}) = \max(\mathbf{y}, 0)$ (projection onto non-negative orthant) where $\mathcal{P}_{\mathbb{R}^n_+}$ is the projection operator.

In fact, this method may produce a bad solution if $\mathbf{x}_{\mathsf{LS}}$ contains many negative parts. This method only works if all the element of $\mathbf{x}_{\mathsf{LS}}$ are non-negative.

Solving NNLS by Projected Gradient Descent

For $f(\mathbf{x}) = \dfrac{1}{2}\mathbf{x}^\top \mathbf{Q}\mathbf{x} - \mathbf{p}^\top \mathbf{x}$, the gradient and the projection are

$$\nabla f = \mathbf{Q}\mathbf{x} - \mathbf{p} \qquad \mathcal{P}_{\mathbb{R}^n_+}(\mathbf{x}) = \max(\mathbf{x}, 0)$$

So the Projected Gradient Descent (PGD) algorithm for solving NNLS is :

Algorithm 1: PGD for NNLS

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)
Initialization Set $\mathbf{x}_0 \in \mathbb{R}^n_+$, $\mathbf{p} = \mathbf{A}^\top \mathbf{b}$, $\mathbf{Q} = \mathbf{A}^\top \mathbf{A}$
while *stopping condition is not met* **do**
  $\mathbf{x}_{k+1} = [\mathbf{x}_k - t_k(\mathbf{Q}\mathbf{x}_k - \mathbf{p})]_+$
end

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where step size t_k can be set as $\frac{1}{L}$, where L is the Lipschitz constant of $\nabla f(\mathbf{x})$.
Next slide tells L of f is $\|\mathbf{Q}\|_2$.

A lemma

Fact 1. For a matrix $\mathbf{A}$ and a vector $\mathbf{x}$, we have $\|\mathbf{A}\mathbf{x}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2$.
Remark : this is operator norm inequality, which is a immediate consequence of the definition of operator norm.

Lemma 1. $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2$ is L-smooth with $L = \|\mathbf{A}^\top \mathbf{A}\|_2$.

i.e. $\|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\|_2 \leq L\|\mathbf{x}_1 - \mathbf{x}_2\|_2$ and $L = \|\mathbf{Q}\|_2 = \|\mathbf{A}^\top \mathbf{A}\|_2$.

Proof. Direct proof.

$$\begin{aligned}
\|\nabla f(\mathbf{x}_1) - \nabla f(\mathbf{x}_2)\|_2 &= \|(\mathbf{A}^\top \mathbf{A}\mathbf{x}_1 - \mathbf{A}^\top \mathbf{b}) - (\mathbf{A}^\top \mathbf{A}\mathbf{x}_2 - \mathbf{A}^\top \mathbf{b})\|_2 \\
&= \|\mathbf{A}^\top \mathbf{A}\mathbf{x}_1 - \mathbf{A}^\top \mathbf{A}\mathbf{x}_2\|_2 \\
&= \|\mathbf{A}^\top \mathbf{A}(\mathbf{x}_1 - \mathbf{x}_2)\|_2 \\
&\overset{\text{fact 1}}{\leq} \|\mathbf{A}^\top \mathbf{A}\|_2 \|\mathbf{x}_1 - \mathbf{x}_2\|_2 \qquad \square
\end{aligned}$$

Soving NNLS by PGD

With $L = \|\mathbf{A}^\top\mathbf{A}\|_2$, step size $t = \dfrac{1}{L} = \dfrac{1}{\|\mathbf{A}^\top\mathbf{A}\|_2}$, the PGD algorithm for solving NNLS becomes:

Algorithm 2: PGD (constant step size) for NNLS

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)

Initialization Set $\mathbf{x}_0 \in \mathbb{R}^n_+$, $\mathbf{p} = \mathbf{A}^\top\mathbf{b}$, $\mathbf{Q} = \mathbf{A}^\top\mathbf{A}$, $t = \dfrac{1}{\|\mathbf{Q}\|_2}$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\mathbf{x}_k - t(\mathbf{Q}\mathbf{x}_k - \mathbf{p})]_+$

end

From the theory of gradient descent, PGD converges at rate $\mathcal{O}(\frac{1}{k})$, where k is the iteration number.

Implementation issue – more compact form

The update re-written in a more compact form is

$$\mathbf{x}_{k+1} = \left[(\mathbf{I}_n - t\mathbf{Q})\mathbf{x}_k + t\mathbf{p}\right]_+$$

Fix constants can be pre-computed outside the loop, we have

Algorithm 3: PGD (constant step size) for NNLS (compact form)

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)

Initialization Set $\mathbf{x}_0 \in \mathbb{R}^n_+$, $\Theta_1 = \mathbf{I}_n - \dfrac{\mathbf{A}^\top\mathbf{A}}{\|\mathbf{A}^\top\mathbf{A}\|_2}$, $\theta_2 = \dfrac{\mathbf{A}^\top\mathbf{b}}{\|\mathbf{A}^\top\mathbf{A}\|_2}$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\Theta_1\mathbf{x}_k + \theta_2]_+$

end

Nesterov's acceleration can be use.
The accelerated PGD (APGD, with constant step size) algorithm is

Algorithm 4: APGD for NNLS

Result: A solution $\mathbf{x}$ that approximately solves NNLS$(\mathbf{A},\mathbf{b})$

Initialization Set $\mathbf{y}_0 = \mathbf{x}_0 \in \mathbb{R}^n_+$, $\Theta_1 = \mathbf{I}_n - \dfrac{\mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}^\top \mathbf{A}\|_2}$, $\theta_2 = \dfrac{\mathbf{A}^\top \mathbf{b}}{\|\mathbf{A}^\top \mathbf{A}\|_2}$

Set $\alpha_1 \in (0\ 1)$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\Theta_1 \mathbf{y}_k + \theta_2]_+$ (projected gradient step)

$\quad \alpha_{k+1} = \frac{1}{2}(\sqrt{\alpha_k^4 + 4\alpha_k^2} - \alpha_k^2)$, $\beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2 + \alpha_{k+1}}$ (Nesterov's parameters)

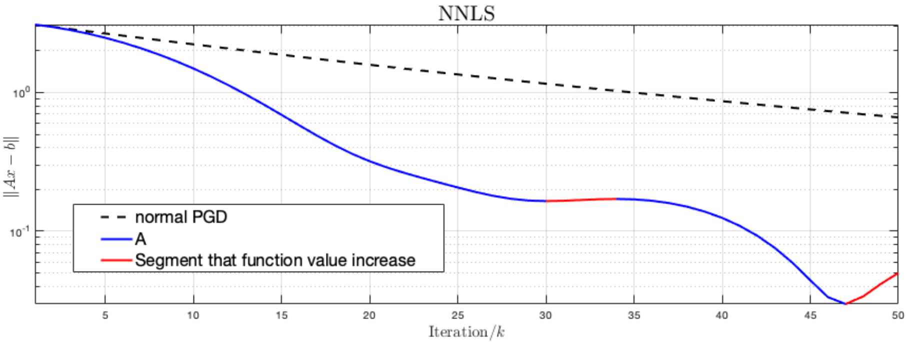
$\quad \mathbf{y}_{k+1} = \mathbf{x}_{k+1} + \beta_k(\mathbf{x}_{k+1} - \mathbf{x}_k)$ (extrapolation)

end

The items in blue are the modifications from Nesterov's acceleration.

PGD is monotone but APGD is not

Recall, PGD is a *monotone*[1] method : for all k, $f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k)$.
However, Nesterov's acclerated method is not monotone : at certain iteration, it is possible the objective value actually increases.



An illustrative example $(m, n) = 100, 5$.

[1]In Nesterov's wording, relaxation sequence.

Accelerated Projected Gradient Descent with restart

To make the scheme monotone, we can apply *adaptive restart* : if error increases, we switch to gradient descent, and reset all parameters.

Algorithm 5: APGD for NNLS

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)

Initialization Set $\mathbf{y}_0 = \mathbf{x}_0 \in \mathbb{R}^n_+$, $\Theta_1 = \mathbf{I}_n - \dfrac{\mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}^\top \mathbf{A}\|_2}$, $\theta_2 = \dfrac{\mathbf{A}^\top \mathbf{b}}{\|\mathbf{A}^\top \mathbf{A}\|_2}$

Set $\alpha_1 \in (0\ 1)$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\Theta_1 \mathbf{y}_k + \theta_2]_+$ (projected gradient step)

$\quad \alpha_{k+1} = \frac{1}{2}(\sqrt{\alpha_k^4 + 4\alpha_k^2} - \alpha_k^2)$, $\beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2 + \alpha_{k+1}}$ (acceleration parameter)

$\quad \mathbf{y}_{k+1} = \mathbf{x}_{k+1} + \beta_k(\mathbf{x}_{k+1} - \mathbf{x}_k)$ (extrapolation)

$\quad$ **if** error increases **do**

$\quad\quad \mathbf{x}_{k+1} = [\Theta_1 \mathbf{x}_k + \theta_2]_+$ (perform normal projected gradient step)

$\quad\quad \mathbf{y}_{k+1} = \mathbf{x}_{k+1}$ (re-start)

$\quad\quad \alpha_k = \alpha_1$ (reset all parameter)

end

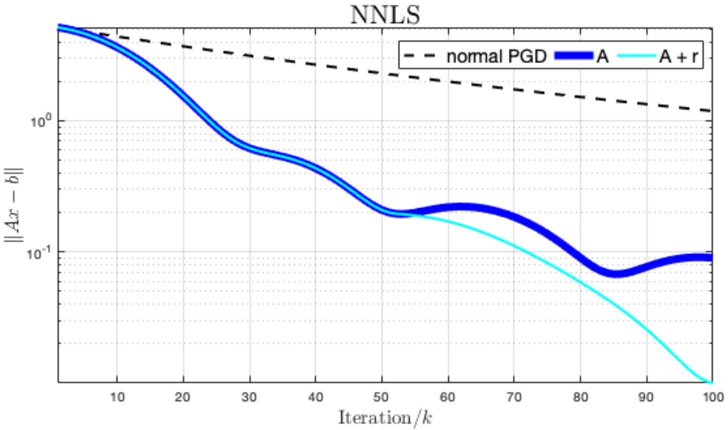


Figure: An illustrative example $(m, n) = 100, 10$.

MATLAB code (click me)

Nesterov's Acceleration other β

In fact the acceleration parameter

$$\alpha_{k+1} = \frac{1}{2}\left(\sqrt{\alpha_k^4 + 4\alpha_k^2} - \alpha_k^2\right), \quad \beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2 + \alpha_{k+1}}$$

are not directly come from the original paper of Nesterov. They come from FISTA. Furthermore, the equations of the parameters are so "complicated". Is there a simpler one ?

In fact, yes. Paul Tseng gave $\beta_k = \dfrac{k-1}{k+2}$:

Algorithm 6: APGD for NNLS using Paul Tseng's β

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)

Initialization Set $\mathbf{y}_0 = \mathbf{x}_0 \in \mathbb{R}^n_+$, $\Theta_1 = \mathbf{I}_n - \dfrac{\mathbf{A}^\top\mathbf{A}}{\|\mathbf{A}^\top\mathbf{A}\|_F}$, $\theta_2 = \dfrac{\mathbf{A}^\top\mathbf{b}}{\|\mathbf{A}^\top\mathbf{A}\|_F}$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\Theta_1\mathbf{y}_k + \theta_2]_+$ (projected gradient step)

$\quad \mathbf{y}_{k+1} = \mathbf{x}_{k+1} + \dfrac{k-1}{k+2}(\mathbf{x}_{k+1} - \mathbf{x}_k)$ (extrapolation)

end

APGD with constant β

Note that the function $f(\mathbf{x})$ in NNLS is smooth and strongly convex.

- Strongly convex
  Recall : a function $f(\mathbf{x})$ is strongly convex iff $\nabla^2 f(\mathbf{x}) - \mu\mathbf{I} \geq 0$.
  As $\nabla^2 f(\mathbf{x}) = \mathbf{Q} = \mathbf{A}^\top \mathbf{A}$, hence we have
  $$\mathbf{Q} - \mu\mathbf{I} \geq 0.$$
  Here, μ can be taken as $\lambda_{\text{min}}(\mathbf{Q}) = \sigma_{\text{min}}(\mathbf{A})$.
- L-Smooth
  As f is twice differentiable, f is L-smooth iff $\nabla^2 f(\mathbf{x}) - L\mathbf{I} \leq 0$.
  Then we have $L \leq \lambda_{\text{max}}(\mathbf{Q}) = \sigma_{\text{max}}(\mathbf{A})$.

For smooth strongly convex function, the extrapolation parameter β of Nesterov's acceleration can be set as follows

$$\beta_k = \beta = \frac{1 - \sqrt{Q}}{1 + \sqrt{Q}}$$

where $Q = \dfrac{L}{\mu}$ is the (optimization) conditional number of the f.

Recall the (linear algebra) conditional number of a matrix $\mathbf{A}$ is $\kappa(\mathbf{A})$.

With constant β, we have the following

Algorithm 7: APGD for NNLS using fixed β

Result: A solution $\mathbf{x}$ that approximately solves NNLS($\mathbf{A}$,$\mathbf{b}$)

Initialization Set $\mathbf{y}_0 = \mathbf{x}_0 \in \mathbb{R}^n_+$, $\Theta_1 = \mathbf{I}_n - \dfrac{\mathbf{A}^\top \mathbf{A}}{\|\mathbf{A}^\top \mathbf{A}\|_F}$, $\theta_2 = \dfrac{\mathbf{A}^\top \mathbf{b}}{\|\mathbf{A}^\top \mathbf{A}\|_F}$

Set $\beta = \dfrac{1-\sqrt{\kappa}}{1+\sqrt{\kappa}}$, where $\kappa = \dfrac{L}{\mu} = \dfrac{\lambda_{\text{max}}(\mathbf{Q})}{\lambda_{\text{min}}(\mathbf{Q})} = \dfrac{\sigma_{\text{max}}(\mathbf{A})}{\sigma_{\text{min}}(\mathbf{A})} = \dfrac{1}{\kappa(\mathbf{A})}$

while *stopping condition is not met* **do**

$\quad \mathbf{x}_{k+1} = [\Theta_1 \mathbf{y}_k + \theta_2]_+$ (projected gradient step)

$\quad \mathbf{y}_{k+1} = \mathbf{x}_{k+1} + \beta_k(\mathbf{x}_{k+1} - \mathbf{x}_k)$ (extrapolation)

end

The items in blue are the modifications from the acceleration scheme with fixed β.

Comparisons

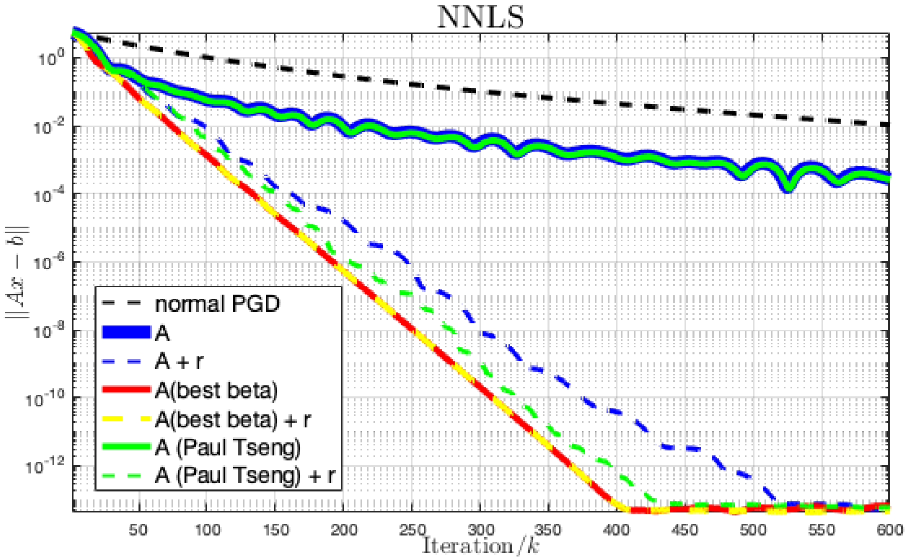


Figure: An illustrative example $(m, n) = 100, 20$. MATLAB code (click me)

Last page - summary

Summary :

- NNLS problem $\min_{\mathbf{x}\in\mathbb{R}^n_+} f(\mathbf{x}) = \frac{1}{2}\|\mathbf{A}\mathbf{x}-\mathbf{b}\|_2^2$
- PGD algorithm for NNLS
- APGD algorithms for NNLS
- APGD algorithm with restart for NNLS

Not discussed :

- Second order methods
- Active set methods

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