Multiplicative Updates for Nonnegative Least Squares

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Joint work with Matt Brand, Mitsbushi Electronic Research Lab *what really matters is the wisdom he teaches you, ...*

– Sofia Pauca

Outline

Objective function

Nonnegative Least Squares

$$\underset{x}{\operatorname{argmin}}\ F(x) = \underset{x}{\operatorname{argmin}}\ ||Ax - b||_2^2 \quad s.t. \quad x \geq 0, \tag{1}$$

Objective function

Nonnegative Least Squares

$$\underset{x}{\operatorname{argmin}}\ F(x) = \underset{x}{\operatorname{argmin}}\ ||Ax - b||_2^2 \quad s.t. \quad x \geq 0, \tag{1}$$

Because

$$\begin{aligned} ||Ax - b||_2^2 &= (Ax - b)^T(Ax - b) \\ &= x^T(A^TA)x - \underbrace{b^T(Ax)}_{\text{scalar}} - \underbrace{(Ax)^Tb}_{\text{scalar}} + \underbrace{b^Tb}_{\text{constant}} \\ &= x^T(A^TA)x - x^T(A^Tb) - x^T(A^Tb) + b^Tb \\ &= x^T(A^TA)x - 2x^T(A^Tb) + b^Tb \end{aligned}$$

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&= x^T(A^TA)x - \underbrace{b^T(Ax)}_{\text{scalar}} - \underbrace{(Ax)^Tb}_{\text{scalar}} + \underbrace{b^Tb}_{\text{constant}} \\
&= x^T(A^TA)x - x^T(A^Tb) - x^T(A^Tb) + b^Tb \\
&= x^T(A^TA)x - 2x^T(A^Tb) + b^Tb
\end{aligned}$$

Hence, solving Equation (1) is equivalent to solving

$$\operatorname*{argmin}_x F(x) = \operatorname*{argmin}_x \frac{1}{2}x^TQx - x^Th \quad s.t. \quad x \geq 0, \tag{2}$$

with $Q = A^TA$ and $h = A^Tb$.

Multiplicative NNLS Iteration

Theorem (Multiplicative NNLS Iteration)

Nonnegative least squares objective function $F(x)$ *in Equation* (2) *is monotonically decreasing under the multiplicative update*

$$x_i^{k+1} = x_i^k \left[\frac{2(Q^- x^k)_i + h_i^+ + \delta}{(|Q| x^k)_i + h_i^- + \delta} \right], \tag{3}$$

with $\delta > 0$, $Q^- = -\min(Q, 0)$, $|Q| = \mathit{abs}(Q)$, $h^+ = \max(h, 0)$, $h^- = -\min(h, 0)$.

M. E. Daube-Witherspoon, G. Muehllehner, in *IEEE Trans. on Medical Imaging*, 1986.

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with $\delta > 0$, $Q^- = -\min(Q, 0)$, $|Q| = \textit{abs}(Q)$, $h^+ = \max(h, 0)$, $h^- = -\min(h, 0)$.

Remark: If Q and h have only nonnegative components and $\delta = 0$, above iteration reduces to

$$x_i^{k+1} = x_i^k \left[\frac{h_i}{(Qx^k)_i} \right],$$

which is called image space reconstruction algorithm (ISRA). Lee ad Seung generalize the ISRA idea to NMF.

M. E. Daube-Witherspoon, G. Muehllehner, in *IEEE Trans. on Medical Imaging*, 1986.

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Gradient Descent Property

The multiplicative update (3) is an element-wise iterative gradient descent method.

$$
\begin{aligned}
x_i^{k+1} - x_i^k &= \left[\frac{2(Q^- x^k)_i + h_i^+ + \delta}{(|Q|x^k)_i + h_i^- + \delta}\right] x_i^k - x_i^k \\
&= \left[\frac{2(Q^- x^k)_i + h_i^+ - (|Q|x^k)_i - h_i^-}{(|Q|x^k)_i + h_i^- + \delta}\right] x_i^k \\
&= -\left[\frac{(Qx^k)_i - h_i}{(|Q|x^k)_i - h_i^- + \delta}\right] x_i^k \\
&= -\left[\frac{x_i^k}{(|Q|x^k)_i - h_i^- + \delta}\right] ((Qx^k)_i - h_i) \\
&= -\gamma_k \nabla(F(x^k)),
\end{aligned}
$$

where the step-size $\gamma_k = \left[\frac{x_i^k}{(|Q|x^k)_i - h_i^- + \delta}\right]$, and $\nabla(F(x)) = Qx^k - h$.

What if $\delta = 0$?

Suppose

$$Q = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad h = 0,$$

with initial guess,

$$\begin{aligned} x^0 &= (\frac{2}{3}, \frac{4}{3}), \\ x^1 &= (\frac{4}{3}, \frac{2}{3}), \\ x^2 &= (\frac{2}{3}, \frac{4}{3}), \quad \cdots \end{aligned}$$

However, the optimal solution is

$$x^* = (r, r), r \in \mathcal{R}.$$

iterations by (3) with $\delta = 0$

Positive δ

Suppose

$$Q = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad h = 0,$$

with initial guess,

$$\begin{aligned} x^0 &= (\frac{2}{3}, \frac{4}{3}), \\ &\vdots \\ x^\infty &= (1, 1), \end{aligned}$$

iterations by (3) with $\delta = 1$

Convergence Analysis

Definition (Auxiliary Function)

For positive vectors, x, y, an auxiliary function, $G(x, y)$, of $F(x)$, has the following two properties

- $F(x) < G(x, y)$ *if* $x \neq y$;
- $F(x) = G(x, x)$

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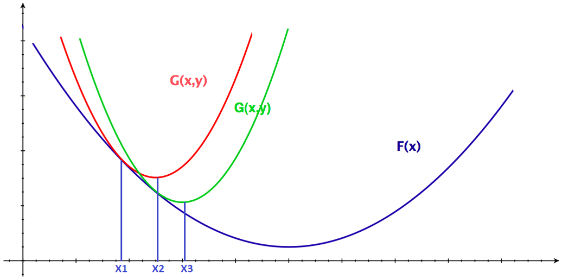

Convergence Analysis contd.

Lemma

Assume $G(x, y)$ *is an auxiliary function of* $F(x)$*, then* $F(x)$ *is strictly decreasing under the update*

$$x^{k+1} = \operatorname*{argmin}_x G(x, x^k),$$

if and only if $x^{k+1} \neq x^k$.

Convergence Analysis contd.

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Proof:
By the definition of an auxiliary function $G(x, y)$, if $x^{k+1} \neq x^k$, we have

$$F(x^{k+1}) < G(x^{k+1}, x^k) \leq G(x^k, x^k) = F(x^k).$$

The equality attains if and only if $x^{k+1} = x^k$.

□

Convergence Analysis contd.

Lemma

For any positive vectors, x, y, *define the diagonal matrix,* $D(y)$, *with diagonal element*

$$D_{ii} = \frac{(|Q|y)_i + h_i^- + \delta}{y_i}, \quad i = 1, 2, \cdots, n$$

where $\delta > 0$. *The function*

$$G(x, y) = F(y) + (x - y)^T \nabla F(y) + \frac{1}{2}(x - y)^T D(y)(x - y)$$

is an auxiliary function for

$$F(x) = \frac{1}{2}x^T Qx - x^T h.$$

Review

Theorem (Multiplicative NNLS Iteration)

Nonnegative least squares objective function $F(x)$

$$\underset{x}{\operatorname{argmin}}\ F(x) = \underset{x}{\operatorname{argmin}}\ \frac{1}{2} x^T Q x - x^T h \quad s.t. \quad x \geq 0,$$

is monotonically decreasing under the multiplicative update

$$x_i^{k+1} = x_i^k \left[\frac{2(Q^- x^k)_i + h_i^+ + \delta}{(|Q| x^k)_i + h_i^- + \delta} \right],$$

with $\delta > 0$, $Q^- = -\min(Q, 0)$, $|Q| = \textit{abs}(Q)$, $h^+ = \max(h, 0)$, $h^- = -\min(h, 0)$.

Review contd.

Suppose

$$Q = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad h = 0,$$

with initial guess,

$$\begin{aligned} x^0 &= (\frac{2}{3}, \frac{4}{3}), \\ &\vdots \\ x^\infty &= (1, 1), \end{aligned}$$

iterations by (3) with $\delta = 1$

Sparse Solution?

If a sparse solution is expected, it is recommended to add a regularization term to the original least squares problem,

$$\underset{x}{\operatorname{argmin}}\ \hat{F}(x) = \underset{x}{\operatorname{argmin}}\ ||Ax - b||_2^2 + \lambda||x||_1, \quad x \geq 0, \lambda > 0 \qquad (4)$$

with nonnegative λ as the regularization parameter.

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with nonnegative λ as the regularization parameter.

Theorem

The objective function $\hat{F}(x)$ in (4) is monotonically decreasing under the multiplicative update

$$x_i^{k+1} = x_i^k \left[\frac{2(Q^- x^k)_i + h_i^+}{(|Q|x^k)_i + h_i^- + \lambda} \right], \qquad (5)$$

with $\lambda > 0$.

Sparse Solution cont.

Suppose

$$Q = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad h = 0,$$

with initial guess,

$$\begin{aligned} x^0 &= (\frac{2}{3}, \frac{4}{3}), \\ &\vdots \\ x^\infty &= (0, 0), \end{aligned}$$

iterations by (5) with $\lambda = 2$

Image Labelling

$$f(x) := \sum_{a=1}^{K} \sum_{i} \left(\frac{\eta}{2} \sum_{j \in \mathcal{N}(i)} \omega_{ij} (x_{ia} - x_{ja})^2 + d_{ia} x_{ia} \right)$$

with constraints

$$\forall i, \quad \sum_{a=1}^{K} x_{ia} = 1, \quad x_{ia} \geq 0,$$

- x_{ia} is the probability of pixel i belongs to labelling set a
- K is the number of labelling sets
- ω_{ij} is the weight between adjacent pixel i and j,

$$\omega_{ij} := \frac{I_i^T I_j}{|I_i| \cdot |I_j|} = \cos(\theta),$$

  where $I.$ is the image value
- $\mathcal{N}(i)$ represents the neighbours of pixel i
- η is a parameter controlling the spatial smoothness
- d_{ia} is the cost of label a at each pixel

M. Rivera, O. Dalmau, and J. Tago, in *ICPR*, pp.1-5, 2008.

Image Labelling: Matrix d

- Mixture Gaussian
  - Assume the data points were drawn from N independent Gaussian distributions with mean μ_l and covariance Σ_l.
  - Compute the Mahalanobis distance between each pixel i and these Gaussian distributions.

$$d_{ia} = \sum_l (x_i - \mu_{la})^T \Sigma_{la}^{-1} (x - \mu_{la}) + \log(\Sigma_{la})$$

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- Support Vector Machine (SVM)
  - Using SVM to find the support vectors for each labelling set.
  - Compute the decision function.

$$d_{ia} = \sum_l \alpha_{la} K(x_i, SV_{ia}) + b_a,$$

where $K(*,*)$ is the kernel function in SVM, α_{la} is the coefficients, and b_a is the bias for labelling set a.

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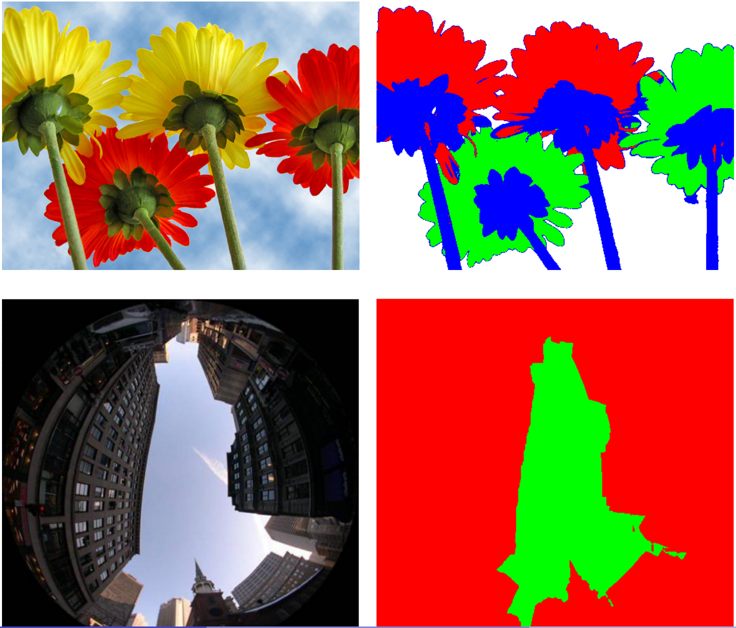
Image Labelling contd.



Conclusion

Introduced a new algorithm along with its convergence analysis for the NNLS problem

$$\underset{x}{\operatorname{argmin}}\ F(x) = \underset{x}{\operatorname{argmin}}\ ||Ax - b||_2^2 \quad s.t. \quad x \geq 0,$$

$$x_i^{k+1} = x_i^k \left[\frac{2(Q^- x^k)_i + h_i^+ + \delta}{(|Q|x^k)_i + h_i^- + \delta} \right],$$

where $Q = A^T A$ and $h = A^T b$.

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