ℓ_1 -NMF for Sparse Data

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Summary

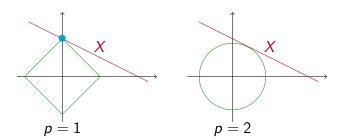
- 1 Known facts about the ℓ_1 -norm in optimization
- 2 What we want to do
- 3 The ℓ_1 -NMF model o our problem
- 4 How to update?
- 5 How to initialize?
- 6 Some numerical experiments
- 7 Conclusion and perspectives

- **1** Known facts about the ℓ_1 -norm in optimization
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The ℓ_1 -norm induces sparsity

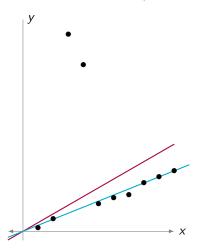
$$\min_{x} \|x\|_{p}$$

s.t. $x \in X$



The ℓ_1 -norm has a special shape: it has spikes at sparse points.

The ℓ_1 -norm is more robust to outliers Given *n* points (x_i, y_i) , we want to fit the model $y = \alpha x$.



For
$$\ell_2$$
-norm, $\alpha^* = \arg\min_{\alpha} (y_1 - \alpha x_1)^2 + ... + (y_n - \alpha x_n)^2 = \arg\min_{\alpha} \|y - \alpha x\|_2$.
For ℓ_1 -norm, $\alpha^* = \arg\min_{\alpha} |y_1 - \alpha x_1| + ... + |y_n - \alpha x_n| = \arg\min_{\alpha} \|y - \alpha x\|_1$.

Focus on these 1-variable problems

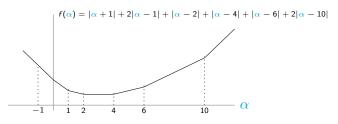
Given $x, y \in \mathbb{R}^n$, find $\alpha \in \mathbb{R}$ s.t. αx is as close as possible to y.

■ With the ℓ_2 -norm, solving min $\|y - \alpha x\|_2^2$ is a quadratic problem:

$$\alpha^* = \frac{x^T y}{\|x\|_2^2}.$$

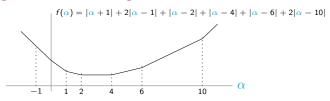
■ With the ℓ_1 -norm, $f(\alpha) = \|y - \alpha x\|_1$ is a sum of absolute values:

$$f(\alpha) = |y_1 - \alpha x_1| + \ldots + |y_n - \alpha x_n| = |x_1| \left| \frac{y_1}{x_1} - \alpha \right| + \ldots + |x_n| \left| \frac{y_n}{x_n} - \alpha \right|.$$



 $\rightarrow \alpha^*$ is at one of the breakpoints $\frac{y_i}{x_i}$.

The weighted median algorithm



How to find α^* ?

- Brute-force: $\mathcal{O}(n^2)$ (n breakpoints to evaluate in $\mathcal{O}(n)$)
- ullet $\mathcal{O}(n)$ algorithm related to the median of medians (but unpractical)
- The weighted median algorithm running in $\mathcal{O}(n \log(n))$:

```
Data: x \in \mathbb{R}^n, y \in \mathbb{R}^n

Result: \arg \min_{\alpha} \sum_{i=1}^n |y_i - \alpha x_i| (w.l.o.g., we suppose x_i > 0 for all i)

[S, indices] \leftarrow \operatorname{sort}\left(\left\{\frac{y_i}{x_i}\right\}\right);

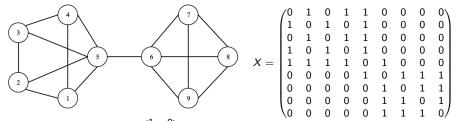
x \leftarrow x(indices);

t \leftarrow \operatorname{smallest} index such that \sum_{i=1}^t x_i \geq \frac{1}{2} \sum_{i=1}^n x_i;

return S_t;
```

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Communities and clusters identification via Matrix Factor.



$$\rightarrow W = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} H = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix}$$

A model/method taking into account the following properties:

- Large-scale data
- Sparse data
- Laplacian noise / Binary noise

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The ℓ_1 -NMF model

Given a matrix
$$X \in \mathbb{R}^{m \times n}$$
,

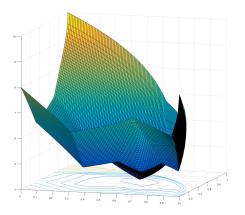
$$\min_{W \ge 0, H \ge 0} \|X - WH\|_1 = \sum_{i=1}^m \sum_{j=1}^n |X - WH|_{ij}.$$

Examples with r = 1:

- This model is much more robust to outliers and non-Gaussian noise
- NP-hard even for r=1

Picture in the rank-1 case

Let us consider the
$$\ell_1$$
-NMF model with $r=1$ for $X=\begin{pmatrix}1&3&1\\1&1&1\\3&1&1\end{pmatrix}$.



Three local minima: $(\frac{3}{\sqrt{11}}, \frac{1}{\sqrt{11}})$, $(\frac{1}{\sqrt{11}}, \frac{1}{\sqrt{11}})$ and $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$ which is the only global min.

Main contribution: an algorithm for the ℓ_1 -NMF model

As for the ℓ_2 -norm, the general problem in both W and H is nonconvex

$$\min_{W\geq 0, H\geq 0}\|X-WH\|_1.$$

but when one of the two factors is given, the subproblems becomes convex :

$$\min_{W\geq 0}\|X-WH\|_1 \qquad \quad \min_{H\geq 0}\|X-WH\|_1.$$

```
 \begin{aligned} \mathbf{Data:} \ & X \in \mathbb{R}_+^{m \times n} \ \text{and factorization rank } k. \\ \mathbf{Result:} \ & (W, H) \geq 0: \ \text{a rank-} r \ \ell_1\text{-NMF of } X \approx WH \\ & (W^{(0)}, H^{(0)}) \geq 0 \leftarrow \text{initialization step;} \\ \mathbf{for} \ & k = 1, 2, \dots \ \mathbf{do} \\ & & H^{(k)} \leftarrow \text{update} \Big(X, W^{(k-1)}\Big) \ ; \\ & & W^{(k)^T} \leftarrow \text{update} \ \Big(X^T, H^{(k-1)^T}\Big) \ ; \end{aligned}
```

end

In the following:

- how to update?
- how to initialize ?

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How to update? Not exactly.

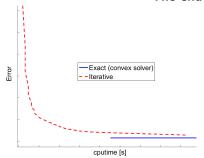
The update of one factor can be separated into n independent subproblems

$$\min_{H\geq 0} \|X - WH\|_1 \quad \to \quad \min_{H(:,j)\geq 0} \sum_{j=1}^n \|X(:,j) - WH(:,j)\|_1,$$

each of them is a convex problem, which can be modelized as an LP

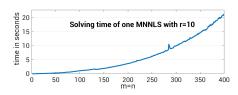
$$\min_{\mathbf{x} \geq 0} \|A\mathbf{x} - b\|_{1} \rightarrow \begin{pmatrix} \min_{\mathbf{x} \geq 0, t} t_{1} + \dots + t_{m} \\ \begin{pmatrix} -A & I \\ A & I \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ t \end{pmatrix} \leq \begin{pmatrix} -b \\ b \end{pmatrix}.$$

The end of the story? No.



No need to update exactly the factors:

- alternate scheme
- cost



How to update? One coordinate at a time.

The idea is to update iteratively the coordinates x_1 , x_2 , ... x_r . For the kth coordinate, the objective function becomes:

$$\min_{\mathbf{x}_{k}\geq 0}\|A\mathbf{x}-b\|_{1} \rightarrow \min_{\mathbf{x}_{k}\geq 0}\left\|A(:,k)\mathbf{x}_{k}-\left(b-\sum_{i\neq k}A(:,i)\mathbf{x}_{i}\right)\right\|_{1},$$

which is exactly the 1-variable problem $\min_{\alpha \geq 0} \|y - \alpha x\|_1$.

Considering the update of the kth entry of the jth column of H, we have:

$$\min_{\boldsymbol{H}_{kj}\geq 0} \left\| W(:,k)\boldsymbol{H}_{kj} - \left(X(:,j) - \sum_{i\neq k} W(:,i)H_{ij} \right) \right\|_{1}.$$

- If the residual $X(:,j) \sum_{i \neq k} W(:,i)H_{ij}$ is available in $\mathcal{O}(m)$, there is an $\mathcal{O}(m)$ algorithm to find the optimal value of H_{ki}
- Overall, updating once every entry of H takes O(mnr) operations

A first algorithm running in $\mathcal{O}(mnr)$ operations

```
Data: X \in \mathbb{R}^{m \times n}, W \in \mathbb{R}_{+}^{m \times r}, H_0 \in \mathbb{R}_{+}^{r \times n}
Result: H \in \mathbb{R}^{r \times n}_{+}
H \leftarrow H_0:
for j = 1 : n \text{ do}
      v = WH(:,j) (\mathcal{O}(mr) oper.);
      for k = 1 : r do
           x = W(:, k);
           y = X(:, j) - v + W(:, k)H_{k,j} (O(m) oper.);
           H_{k,i}^+ \leftarrow \mathtt{weighted\_median}(x,y) \quad (\mathcal{O}(m) \text{ oper.}) ;
         v \leftarrow v + W(:,k)(H_{k,i}^+ - H_{k,i}^{old}) (\mathcal{O}(m) oper.);
      end
```

- The residual is available in $\mathcal{O}(m)$, it allows to update one factor in $\mathcal{O}(mnr)$
 - But, unlike HALS for the ℓ₂-norm, it is not obvious to use the fact that X can be sparse

end

First advantage: modif. to scale with sparse matrices

Let
$$\mathcal{K}^+=\{i\mid X_{i,j}>0\}$$
 and $\mathcal{K}^0=\{i\mid X_{i,j}=0\}$ such that $\mathcal{K}^+\cup\mathcal{K}^0=\{1,...,m\}.$

The objective function becomes:

$$\begin{aligned} & \left\| W(:,k) \mathbf{H}_{kj} - \left(X(:,j) - \sum_{i \neq k} W(:,i) H_{ij} \right) \right\|_{1} \\ &= \left\| W(\mathcal{K}^{+},k) \mathbf{H}_{kj} - \left(X(\mathcal{K}^{+},j) - \sum_{i \neq k} W(\mathcal{K}^{+},i) H_{ij} \right) \right\|_{1} + \left\| W(\mathcal{K}^{0},k) \mathbf{H}_{kj} + \sum_{i \neq k} W(\mathcal{K}^{0},i) H_{ij} \right\|_{1}. \end{aligned}$$

And since $W \geq 0$ and $H \geq 0$, the 1-variable optimization problem becomes

$$\min_{\boldsymbol{H}_{kj} \geq 0} \left\| W(\mathcal{K}^+, k) \boldsymbol{H}_{kj} - \left(X(\mathcal{K}^+, j) - \sum_{i \neq k} W(\mathcal{K}^+, i) H_{ij} \right) \right\|_1 + \left\| W(\mathcal{K}^0, k) \right\|_1 \boldsymbol{H}_{kj}.$$

- The size of this problem is $|\mathcal{K}^+| + 1$.
- When X is sparse, $|\mathcal{K}^+| \ll m$.

A new version running in $\mathcal{O}(\operatorname{nnz}(X)r)$ operations

```
Data: X \in \mathbb{R}^{m \times n}, W \in \mathbb{R}^{m \times r}_{\perp}, H_0 \in \mathbb{R}^{r \times n}_{\perp}
Result: H \in \mathbb{R}^{r \times n}_{\perp}
H \leftarrow H_0:
nW(k) = ||W(:, k)||_1 for all k = 1, ..., r (\mathcal{O}(mr) oper.);
for i = 1 : n do
      \mathcal{K}^+ = \{i \mid X_{i,i} > 0\}:
       v = W(\mathcal{K}^+,:)H(:,j) (\mathcal{O}(|\mathcal{K}^+|r) oper.);
       for k = 1 \cdot r do
           x = W(\mathcal{K}^+, k);
             v = X(\mathcal{K}^+, i) - v + W(\mathcal{K}^+, k)H_{k,i}
                                                                               (\mathcal{O}(|\mathcal{K}^+|) \text{ oper.});
             c = nW(k) - \|W(\mathcal{K}^+, k)\|_1
                                                                                   (\mathcal{O}(|\mathcal{K}^+|) \text{ oper.});
             H_{k,i}^+ \leftarrow \text{weighted\_median}([x \ c], [y \ 0]) \quad (\mathcal{O}(|\mathcal{K}^+|) \text{ oper.});
            v \leftarrow v + W(\mathcal{K}^+, k)(H_{k,i}^+ - H_{k,i}^{\text{old}})
                                                                                  (\mathcal{O}(|\mathcal{K}^+|) \text{ oper.});
       end
```

end

Updating once every entry of one factor can be done in $\mathcal{O}(\operatorname{nnz}(X)r)$ operations.

Second advantage: when $X, W^{(0)}, H^{(0)}$ are binary

Let's take the update in its elementary form:

$$\begin{aligned} & x = W(:, k) \\ & y = X(:, j) - \sum_{i \neq k} W(:, i) H_{i, j} \\ & H_{k, j}^+ \leftarrow \texttt{weighted_median}(x, y) \end{aligned}$$

and the weighted-median algorithm:

```
Data: x \in \mathbb{R}^m, y \in \mathbb{R}^m

[S, indices] \leftarrow \text{sort}\left(\left\{\frac{y_i}{x_i}\right\}\right);

x \leftarrow x(indices);

t \leftarrow \text{smallest index such that } \sum_{i=1}^t x_i \ge \frac{1}{2} \sum_{i=1}^n x_i;

return \max(0, S_t);
```

- the entries of x belong to $\{0,1\}$
- the entries of y belong to $\{-r+1, -r+2, ..., 0, 1\}$
- the entries of the ratios S belong to $\{-r+1, -r+2, ..., 0, 1\}$
- because of $\max(0, S_t)$, $H_{k,j}^+$ belongs to $\{0, 1\}$

The factors W, H remain binary along the iterations.

Observation: the initialization is important

Let's take the update in its "sparse" form:

$$egin{aligned} x &= W(:,k) \ y &= X(:,j) - \sum_{i
eq k} W(:,i) H_{i,j} \ c &= \|W(:,k)\|_1 - \|W(\mathcal{K}^+,k)\|_1 \ H_{k,j}^+ \leftarrow \mathtt{weighted_median}([x\ c],[y\ 0]) \end{aligned}$$

and the weighted-median algorithm:

```
Data: x \in \mathbb{R}^m, y \in \mathbb{R}^m
[S, indices] \leftarrow sort\left(\left\{\frac{y_i}{x_i}\right\}\right);
x \leftarrow x(indices);
t \leftarrow \text{smallest index such that } \sum_{i=1}^{t} x_i \geq \frac{1}{2} \sum_{i=1}^{n} x_i
return \max(0, S_t);
```

- The ratio $\frac{0}{c} = 0$ is always sorted in first position, that is, $x_1 = c$ and $S_1 = 0$
- Observe that the r.h.s of the inequality is $\frac{1}{2}||W(:,k)||_1$
- If we have $c = \|W(:,k)\|_1 \|W(\mathcal{K}^+,k)\|_1 > \frac{1}{2}\|W(:,k)\|_1$, that is,

$$\|W(\mathcal{K}^+,k)\|_1 \leq \frac{1}{2}\|W(:,k)\|_1,$$

then t = 1 and $H_{k,i}^{+} = 0$.

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How to initialize? Not randomly.

$$W^{(0)} = \begin{pmatrix} 0.28 & 0.35 & 0.73 \\ 0.45 & 0.80 & 0.54 \\ 0.98 & 0.98 & 0.89 \\ 0.82 & 0.49 & 0.25 \\ 0.91 & 0.55 & 0.52 \\ 0.56 & 0.33 & 0.49 \\ 0.86 & 0.94 & 0.93 \\ 0.57 & 0.82 & 0.87 \\ 0.52 & 0.62 & 0.20 \\ 0.62 & 0.83 & 0.68 \end{pmatrix} \\ H^{(0)} = \begin{pmatrix} 0.59 & 0.29 & 0.22 & 0.52 & 0.66 & 0.68 & 0.99 & 0.53 & 0.83 & 0.58 \\ 0.29 & 0.42 & 0.14 & 0.12 & 0.62 & 0.40 & 0.46 & 0.31 & 0.92 & 0.32 \\ 0.22 & 0.20 & 0.53 & 0.17 & 0.56 & 0.44 & 0.82 & 0.54 & 0.79 & 0.84 \end{pmatrix}$$

If we update H, we obtain:

How to update ? Another idea: with the ℓ_2 -norm

$$W^{(0)} = \begin{pmatrix} 1.05 & 0.08 & 0 \\ 1.11 & 0 & 0 \\ 0.10 & 1.03 & 0 \\ 0 & 0.93 & 0 \\ 0.10 & 1.03 & 0 \\ 0 & 0.96 & 0.30 \\ 0 & 0 & 0.74 \\ 0 & 0 & 1.11 \\ 0 & 0 & 1.11 \\ 0.45 & 0 & 0.79 \end{pmatrix} H^{(0)} = \begin{pmatrix} 1 & 0.84 & 0 & 0 & 0.45 & 0 & 0.37 & 0 & 0.03 & 0.03 \\ 0 & 0 & 1 & 1 & 0.48 & 1 & 0.99 & 0 & 0 & 0.17 \\ 0.11 & 0 & 0.002 & 0.002 & 0 & 0.002 & 0 & 0.79 & 1 & 0.86 \end{pmatrix}$$

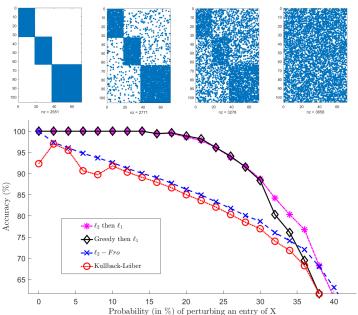
If we update H, we obtain:

How to update? In a greedy way: one rank-1 factor at a time

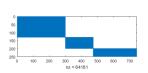
```
 \begin{split} \mathbf{Data} &: X \in \mathbb{R}_+^{m \times n} \quad \mathbf{Result} \colon \ w \in \mathbb{R}_+^m, \ h \in \mathbb{R}_+^n \\ w \leftarrow 0^m \ ; \\ & i^* \leftarrow \arg\max_{i=1,...,m} \|X_{i,:}\|_1 \ ; \\ & w(i^*) \leftarrow 1 \ ; \\ & h \leftarrow X(i^*,:) \ ; \\ & [w,h] \leftarrow \arg\min||X - wh||_1 \ \text{via alternate optimization} \ ; \end{split}
```

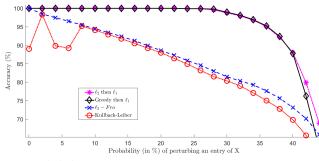
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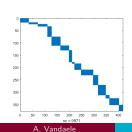
Synthetic datasets

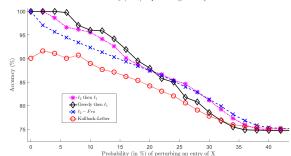


Synthetic datasets









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Conclusion and perspectives

- \blacksquare An algorithm for the $\ell_1\text{-NMF}$ model
- which scales and can handle sparse data
- some pros and cons
- using the ℓ_1 -NMF model is *like doing sparse-NMF*

In the near future:

- not wait 6 months before the next iteration on this work
- convince myself about the greedy initialization (and dig a little deeper)
- more compelling Numerical Experiments section

Thank you! Questions?