A deduction for dictionary learning

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In this article, we would discuss the trick about training and testing phases for dictionary learning (sparse coding). The original work could be referred in [1]. As extra reading materials, we suggest reading [2] for understanding how to apply Lagrangian method and [3] to refer some conclusions about how to calculate gradients for matrices.

1 Solve the Lasso problem

Consider the testing phase of sparse coding which could be formulated as

$$\min_{\{\boldsymbol{\alpha}_i\}_{i=1}^N} \sum_{i=1}^N \left(\|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2 + \lambda \|\boldsymbol{\alpha}_i\|_1 \right).$$
(1-1)

Then we could find the stationary point according to the first-order gradient,

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}_{k}} \left(\sum_{i=1}^{N} \left(\|\mathbf{x}_{i} - \mathbf{D}\boldsymbol{\alpha}_{i}\|_{2}^{2} + \lambda \|\boldsymbol{\alpha}_{i}\|_{1} \right) \right) \\
= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}_{k}} \left(\|\mathbf{x}_{k} - \mathbf{D}\boldsymbol{\alpha}_{k}\|_{2}^{2} + \lambda \|\boldsymbol{\alpha}_{k}\|_{1} \right) \\
= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}_{k}} \left((\mathbf{x}_{k} - \mathbf{D}\boldsymbol{\alpha}_{k})^{T} (\mathbf{x}_{k} - \mathbf{D}\boldsymbol{\alpha}_{k}) \right) + \lambda \mathrm{sign}(\boldsymbol{\alpha}_{k}) \\
= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\alpha}_{k}} \left(-2\boldsymbol{\alpha}_{k}^{T} \mathbf{D}^{T} \mathbf{x}_{k} + \boldsymbol{\alpha}_{k}^{T} \mathbf{D}^{T} \mathbf{D}\boldsymbol{\alpha}_{k} \right) + \lambda \mathrm{sign}(\boldsymbol{\alpha}_{k}) \\
= -2\mathbf{D}^{T} \mathbf{x}_{k} + 2\mathbf{D}^{T} \mathbf{D}\boldsymbol{\alpha}_{k} + \lambda \mathrm{sign}(\boldsymbol{\alpha}_{k}) = 0.$$
(2)

(2) indicates the analytical solution for Lasso problem implicitly. To find the best $\boldsymbol{\alpha}_k$, we still need to apply some tricks. Denote that $\boldsymbol{\theta}_k = \operatorname{sign}(\boldsymbol{\alpha}_k)$, we could rewrite (2) as

$$\boldsymbol{\alpha}_{k} = (\mathbf{D}^{T}\mathbf{D})^{-1}(\mathbf{D}^{T}\mathbf{x}_{k} - \frac{\lambda}{2}\boldsymbol{\theta}_{k}).$$
(3)

Since $\boldsymbol{\theta}_k = \operatorname{sign}(\boldsymbol{\alpha}_k)$, we could apply $\operatorname{sign}(\cdot)$ to both sides of (3), then we get

$$\operatorname{sign}\left(\frac{1}{\lambda}\frac{\mathrm{dLasso}}{\mathrm{d}\boldsymbol{\alpha}_{k}}\right) = \operatorname{sign}\left((\mathbf{D}^{T}\mathbf{D})^{-1}(\mathbf{D}^{T}\mathbf{x}_{k} - \frac{\lambda}{2}\boldsymbol{\theta}_{k})\right) - \boldsymbol{\theta}_{k}$$
$$= \operatorname{sign}\left(\mathbf{D}^{T}\mathbf{x}_{k} - \frac{\lambda}{2}\boldsymbol{\theta}_{k}\right) - \boldsymbol{\theta}_{k}$$
$$= \operatorname{sign}\left(\mathbf{y}_{k} - \lambda\boldsymbol{\theta}_{k}\right) - \boldsymbol{\theta}_{k} = 0.$$
(4)

(4) indicates a fast solution for (2). It proves that considering that the *i*th element of \mathbf{y}_k , i.e. y_{ki} , we would find that when $y_{ki} > \lambda$, $\alpha_{ki} > 0$, and when $y_{ki} < -\lambda$, $\alpha_{ki} < 0$. Furthermore, when $y_{ki} \in [-\lambda, \lambda]$, $\alpha_{ki} = 0$. After confirming $\boldsymbol{\theta}_k$, it will be easy to get $\boldsymbol{\alpha}_k$ from (3) directly.

2 Learn the dictionary

If we rewrite the coding as a matrix as below,

$$\mathbf{A} = \begin{bmatrix} \boldsymbol{\alpha}_1 & \boldsymbol{\alpha}_2 & \cdots & \boldsymbol{\alpha}_N \end{bmatrix}, \tag{5}$$

then we could rewrite the dictionary learning problem by Frobenius norm,

$$\min_{\mathbf{D}} \|\mathbf{X} - \mathbf{D}\mathbf{A}\|_{F}^{2}, \tag{6-1}$$

s.t.
$$||D(:,k)||_2 \leq 1, \ \forall k \in \{1, 2, \dots, K\}.$$
 (6-2)

Training dictionary requires us to train \mathbf{D} and \mathbf{A} alternatively. The method for training \mathbf{A} has been discussed before, hence we would discuss how to train \mathbf{D} in the following part. Subsequently, we only note that the trainable variable is \mathbf{D} (6-1), which means (1-1) and (6-1) require to be solved alternatively.

Solving the dictionary training need us to use Lagrangian multiplier method. Denote the multiplier as μ_j , we could incorporate the constraints into the problem,

$$\mathcal{L}(\mathbf{D}, \ \boldsymbol{\mu}) = \|\mathbf{X} - \mathbf{D}\mathbf{A}\|_{F}^{2} + \sum_{j=1}^{K} \mu_{j} \sum_{i=1}^{D} (D_{ij}^{2} - 1).$$
(7)

The first term of (7) could be expanded as

$$\|\mathbf{X} - \mathbf{D}\mathbf{A}\|_{F}^{2} = \operatorname{Tr}((\mathbf{X} - \mathbf{D}\mathbf{A})(\mathbf{X} - \mathbf{D}\mathbf{A})^{T})$$

= Tr($\mathbf{X}\mathbf{X}^{T}$) + Tr($\mathbf{D}\mathbf{A}\mathbf{A}^{T}\mathbf{D}^{T}$) - 2Tr($\mathbf{D}\mathbf{A}\mathbf{X}^{T}$). (8)

Denote a diagonal matrix Λ where each element is μ_j , Then the second term could be rewritten as

$$\sum_{j=1}^{K} \mu_j \sum_{i=1}^{D} (D_{ij}^2 - 1) = \sum_{j=1}^{K} \mu_j \sum_{i=1}^{D} (D_{ij}^2) - \sum_{j=1}^{K} \mu_j$$

$$= \operatorname{Tr}(\mathbf{D}\mathbf{\Lambda}\mathbf{D}^T - \mathbf{\Lambda}).$$
(9)

Hence we could rewrite (7) as

$$\mathcal{L}(\mathbf{D}, \mathbf{\Lambda}) = \operatorname{Tr}(\mathbf{X}\mathbf{X}^T + \mathbf{D}\mathbf{A}\mathbf{A}^T\mathbf{D}^T - 2\mathbf{D}\mathbf{A}\mathbf{X}^T + \mathbf{D}\mathbf{\Lambda}\mathbf{D}^T - \mathbf{\Lambda}).$$
(10)

Apply the first-order partial gradient to \mathbf{D} , we have

$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{D}} \left(\mathcal{L}(\mathbf{D}, \mathbf{\Lambda}) \right) = \frac{\mathrm{d}}{\mathrm{d}\mathbf{D}} \left(\mathrm{Tr}(\mathbf{D}\mathbf{A}\mathbf{A}^T\mathbf{D}^T - 2\mathbf{D}\mathbf{A}\mathbf{X}^T + \mathbf{D}\mathbf{\Lambda}\mathbf{D}^T) \right)$$
$$= 2\mathbf{D}\mathbf{A}\mathbf{A}^T - 2\mathbf{X}\mathbf{A}^T + 2\mathbf{D}\mathbf{\Lambda} = 0.$$
$$\mathbf{D} = \mathbf{X}\mathbf{A}^T (\mathbf{A}\mathbf{A}^T + \mathbf{\Lambda})^{-1}.$$
(11)

Substitute (11) into (10), we would have

$$\mathcal{L}(\mathbf{\Lambda}) = \min_{\mathbf{D}} \mathcal{L}(\mathbf{D}, \mathbf{\Lambda})$$

= Tr(XX^T + DAA^TD^T - 2DAX^T + DAD^T - A)
= Tr(XX^T + D(AA^T + A)D^T - 2DAX^T - A)
= Tr(XX^T + XA^T(AA^T + A)^{-1}(AA^T + A)(AA^T + A)^{-1}AX^T (12)
- 2XA^T(AA^T + A)^{-1}AX^T - A)
= Tr(XX^T - XA^T(AA^T + A)^{-1}AX^T - A). (12)

Note that **D** has been represented by Λ , we would know that minimizing $\mathcal{L}(\cdot)$ could be applied on Λ solely. Hence we have

$$\frac{\partial \min \mathcal{L}}{\partial \mu_i} = \operatorname{Tr} \left(\frac{\partial \mathbf{X} \mathbf{X}^T}{\partial \mu_i} - \frac{\partial \mathbf{X} \mathbf{A}^T (\mathbf{A} \mathbf{A}^T + \mathbf{\Lambda})^{-1} \mathbf{A} \mathbf{X}^T}{\partial \mu_i} - \frac{\partial \mathbf{\Lambda}}{\partial \mu_i} \right)$$

$$= -\operatorname{Tr} \left(\frac{\partial \mathbf{X} \mathbf{A}^T (\mathbf{A} \mathbf{A}^T + \mathbf{\Lambda})^{-1} \mathbf{A} \mathbf{X}^T}{\partial \mu_i} \right) - 1.$$
(13)

In [3], there has been a conclusion that

$$\operatorname{Tr}\left(\frac{\partial \mathbf{P}^{T}(\mathbf{X}+\mathbf{A})^{-1}\mathbf{P}}{\partial x_{i}}\right) = -\|\mathbf{P}^{T}(\mathbf{X}+\mathbf{A})^{-1}\mathbf{e}_{i}\|_{2}^{2}.$$
 (14)

Apply (14) to (13), we have

$$\frac{\partial \min \mathcal{L}}{\partial \mu_i} = \|\mathbf{X}\mathbf{A}^T(\mathbf{A}\mathbf{A}^T + \mathbf{\Lambda})^{-1}\mathbf{e}_i\|_2^2 - 1 = 0.$$
(15)

(15) is in the quadratic form, hence it is convex and we could find the analytical solution for Λ . Substitute Λ into (11), we would solve \mathbf{D} .

An interesting thing is that if anyone substitute (11) into (15), then it will be

$$\|\mathbf{De}_i\|_2^2 = \|D(:,i)\|_2 = 1,$$
(16)

which shows that the solution revealed in (11) and (15) fulfills the constraints in (6-2) strictly.

References

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- [3] K. B. Petersen, M. S. Pedersen et al., "The matrix cookbook," Technical University of Denmark, vol. 7, no. 15, p. 510, 2008.