

Lagrangian Dual & KKT Conditions

Presentation 2

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Neural Collapse Terminus: A Unified Solution for Class Incremental Learning and Its Variants

Presentation Overview

- ① Recap
- ② Optimization
 - Constrained Optimization
 - Converting Constrained to Unconstrained optimization
- ③ Lagrangian Dual
- ④ KKT Conditions

Recap

We consider the following problem,

$$\begin{aligned} \min_{\mathbf{M}^{(t)}} \quad & \frac{1}{N^{(t)}} \sum_{k=1}^{K^{(t)}} \sum_{i=1}^{n_k} \mathcal{L} \left(\mathbf{m}_{k,i}^{(t)}, \hat{\mathbf{W}}_{\text{ETF}} \right), \quad 0 \leq t \leq T, \\ \text{s.t.} \quad & \|\mathbf{m}_{k,i}^{(t)}\|^2 \leq 1, \quad \forall 1 \leq k \leq K^{(t)}, 1 \leq i \leq n_k, \end{aligned}$$

where,

$\mathbf{m}_{k,i}^{(t)} \in \mathbb{R}^d$: i -th sample of class k in session t feature

n_k : no. of samples in class k

$K^{(t)}$: no. of classes in session t

$N^{(t)} = \sum_{k=1}^{K^{(t)}} n_k$

$\mathbf{M}^{(t)} \in \mathbb{R}^{d \times N^{(t)}}$: collection of $\mathbf{m}_{k,i}^{(t)}$

$K = \sum_{t=0}^T K^{(t)}$

$\hat{\mathbf{W}}_{\text{ETF}} \in \mathbb{R}^{d \times K}$: neural collapse terminus all K

Definition (Simplex Equiangular Tight Frame)

A simplex equiangular tight frame (ETF) refers to a collection of vectors $\{\mathbf{e}_i\}_{i=1}^K$ in \mathbb{R}^d , $d \geq K - 1$, that satisfies:

$$\mathbf{e}_{k_1}^T \mathbf{e}_{k_2} = \frac{K}{K-1} \delta_{k_1, k_2} - \frac{1}{K-1}, \quad \forall k_1, k_2 \in [1, K],$$

where $\delta_{k_1, k_2} = 1$ when $k_1 = k_2$, and 0 otherwise. All vectors have the same ℓ_2 norm and any pair of two different vectors has the same inner product of $-\frac{1}{K-1}$, which is the minimum possible cosine similarity for K equiangular vectors in \mathbb{R}^d .

Theorem

Let $\hat{\mathbf{M}}^{(t)}$ denotes the global minimizer by optimizing the model incrementally from $t = 0$, and we have $\hat{\mathbf{M}} = [\hat{\mathbf{M}}^{(0)}, \dots, \hat{\mathbf{M}}^{(T)}] \in \mathbb{R}^{d \times \sum_{t=0}^T N^{(t)}}$. No matter if \mathcal{L} is CE or misalignment loss, for any column vector $\hat{\mathbf{m}}_{k,i}$ in $\hat{\mathbf{M}}$ whose class label is k , we have:

$$\|\hat{\mathbf{m}}_{k,i}\| = 1, \quad \hat{\mathbf{m}}_{k,i}^T \hat{\mathbf{w}}_{k'} = \frac{K}{K-1} \delta_{k,k'} - \frac{1}{K-1},$$

for all $k, k' \in [1, K]$, $1 \leq i \leq n_k$, where $K = \sum_{t=0}^T K^{(t)}$ denotes the total number of classes of the whole label space, $\delta_{k,k'} = 1$ when $k = k'$ and 0 otherwise, and $\hat{\mathbf{w}}_{k'}$ is the class prototype in $\hat{\mathbf{W}}_{\text{ETF}}$ for class k' .

Types of Optimization

- Unconstrained
 - Easy.
 - High school math. $f' = 0$.
- Constrained
 - Hard.
 - Convert constrained to unconstrained and solve.
 - Our interest.

Constrained Optimization

$$\begin{array}{ll}\min_x & x_1 + x_2 \\ \text{s.t.} & x_1^2 + x_2^2 - 1 \leq 0\end{array}$$

Constrained to Unconstrained

$$\min_x \quad x_1 + x_2 + P(x_1^2 + x_2^2 - 1)$$

$$P(y) = \begin{cases} \infty & \text{if } y > 0 \\ 0 & \text{otherwise} \end{cases}$$

Constrained to Unconstrained

$$\min_x \quad x_1 + x_2 + P(x_1^2 + x_2^2 - 1)$$
$$P(y) = u \times y$$

Constrained to Unconstrained

$$\min_x x_1 + x_2 + P(x_1^2 + x_2^2 - 1)$$
$$P(y) = \max_{u \geq 0} u \times y$$

Constrained to Unconstrained: Primal

$$\min_x x_1 + x_2 + \max_{u \geq 0} u(x_1^2 + x_2^2 - 1)$$
$$\min_x \max_{u \geq 0} x_1 + x_2 + u(x_1^2 + x_2^2 - 1)$$

Constrained to Unconstrained: Lagrangian Dual

$$\max_{u \geq 0} \min_x \underbrace{x_1 + x_2 + u(x_1^2 + x_2^2 - 1)}_{\text{Lagrangian Dual}}$$

Lagrangian Dual: Lets formalize

$$\begin{array}{ll} \min_x & f(x) \\ \text{s.t} & g_i(x) \leq 0 \quad \forall i \in \{1, 2, 3, 4, \dots\} \end{array}$$

Lagrangian Dual: Lets formalize

$$\min_x f(x) + \max_{u_i \geq 0} \sum_i u_i g_i(x)$$

$$\min_x \max_{u_i \geq 0} f(x) + \sum_i u_i g_i(x)$$

$$\max_{u_i \geq 0} \min_x f(x) + \sum_i u_i g_i(x)$$

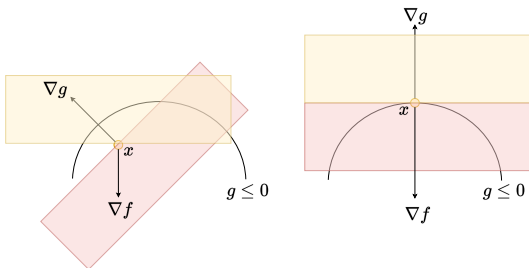
Gradient of Lagrangian

$$\nabla \left(f(x) + \sum_i u_i g_i(x) \right) = 0$$

$$\nabla f(x) + \nabla \left(\sum_i u_i g_i(x) \right) = 0$$

$$\nabla f(x) + u \nabla g(x) = 0$$

$$\nabla f(x) = -u \nabla g(x)$$



KKT Conditions

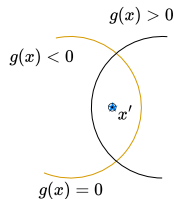
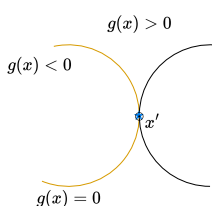
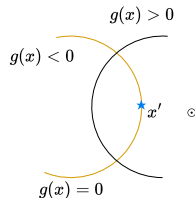
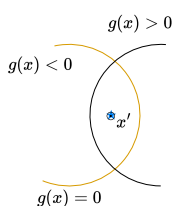
x^* and u^* are values are optimal.

① $\nabla f(x^*) = -u^* \nabla g(x^*)$

② $g(x^*) \leq 0$

③ $u^* \geq 0$

④ $u^* g(x) = 0$



Resources

- <https://www.youtube.com/watch?v=uh1Dk68cfWs>
- https://www.youtube.com/watch?v=s8j-pI_tPlM
- https://www-cs.stanford.edu/people/davidknowles/lagrangian_duality.pdf
- <https://www.youtube.com/watch?v=3ywFQOkzTQE>
- Is there a connection between lagrangian multiplier and eigenvalues? : <https://journeyinmath.wordpress.com/2018/08/18/lagrangemultipliers/>