

A proper way of regularizing DARTS

Department of Computer Engineering

Dongseo University

Jie Yong Shin,

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- 1. Highlights (1)
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- 3. Beta-Decay DARTS (6)
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- 1. Find out the reason why TD-DARTS couldn't improve much compared to DARTS on accuracy
 - Prevent skip connection with Regularization
- 2. Learn an effective way to regularize Differentiable Architecture Search
 - Based on Beta-Decay DARTS
- 3. Observe the difference between Beta-Decay DARTS and other regularization methods

2. Problems of DARTS

Although differentiable method has the advantages of simplicity and computational efficiency, its robustness and architecture generalization challenges still needs to be fully resolved. Firstly, lots of studies have shown that DARTS frequently suffers from performance collapse, that is the searched architecture tends to accumulate parameter-free operations especially for skip connection, leading to the performance degradation [1, 5]. To handle this robustness challenge, lots of instructive works are proposed: directly restricting the number of skip connections [4, 20]; exploiting or regularizing relevant indicators such as the norm of Hessian regarding the architecture parameters [1,3]; changing the searching and/or discretization process [5, 6, 12]; implicitly regularizing the learned architecture parameters [1]. However, the explicit regularization of architecture parameters optimization receives little attention, as previous works (including above methods) adopt L2 or

weight decay regularization by default on learnable architecture parameters (i.e., α), without exploring solution along this direction. Secondly, several works have pointed out that the optimal architecture obtained on the specific dataset cannot guarantee its good performance on another dataset [19,22], namely the architecture generalization challenge. To improve the generalization of searched model, AdaptNAS [19] explicitly minimizes the generalization gap of architectures between domains via the idea of cross domain, MixSearch [22] searches a generalizable architecture by mixing multiple datasets of different domains and tasks. However, both methods solve this issue by leveraging larger datasets, while how to use a single dataset to learn a generalized architecture remains challenging.

Problems

- 1. Discrepancy: Between Continuously encoded architecture and Discrete architecture.
- 2. Performance Collapse: Searched architecture tends to select skip connection.
- 3. Architecture Generalization Challenge: Architecture searched in the specific dataset cannot guarantee it is good also on another dataset.



2. Problem of DARTS



$$\bar{o}^{(i,j)}(x_i) = \sum_{o \in \mathcal{O}} \frac{\exp\left(\alpha_o^{(i,j)}\right)}{\sum_{o' \in \mathcal{O}} \exp\left(\alpha_{o'}^{(i,j)}\right)} o(x_i)$$

Let, Operation Pool = {Convolution(), Pooling(), Skip()}

One-hot encoding:

Operation 1 : Convolution() = [1, 0, 0]

Operation 2 : Pooling() = [0, 1, 0]

Operation 3 : Skip() = [0, 0, 1]

DARTS Assumes that,

 $\alpha_{op1} \approx \text{Convolution()} \approx [1, 0, 0]$

 $\alpha_{op2} \approx \text{Pooling()} \approx [0, 1, 0]$

 $\alpha_{op3} \approx \text{Skip()} \approx [0, 0, 1]$



$$\bar{o}^{(i,j)}(x_i) = \sum_{o \in \mathcal{O}} \frac{\exp\left(\alpha_o^{(i,j)}\right)}{\sum_{o' \in \mathcal{O}} \exp\left(\alpha_{o'}^{(i,j)}\right)} o(x_i)$$

$$\bar{O}^{(i,j)}(x) = \sum_{k=1}^{|\mathcal{O}|} \beta_k^{(i,j)} O_k(x)$$

$$\beta_k^{(i,j)} = \frac{\exp\left(\alpha_k^{(i,j)}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{(i,j)}\right)}$$



$$\alpha = [\alpha_1, \alpha_2, \alpha_3, \cdots, \alpha_k]$$

$$\Upsilon_{1} \simeq OP_{1}$$

$$OP_1 = [1, 0, 0, \cdots, 0]$$



$$\beta_{k} = \frac{Q^{\gamma_{k}}}{\sum_{k'=1}^{|Q|} Q^{\gamma_{k'}}}$$





$$\beta_{3} = \frac{\left[\alpha_{1}, \alpha_{2}, \alpha_{3}\right]}{\left[\alpha_{1} + \alpha_{2} + \alpha_{3}\right]},$$

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$$\beta_{3} = \frac{\left[\alpha_{1} + \alpha_{2} + \alpha_{3}\right]}{\left[\alpha_{1} + \alpha_{2} + \alpha_{3}\right]},$$

$$\therefore \geq \beta = 1$$



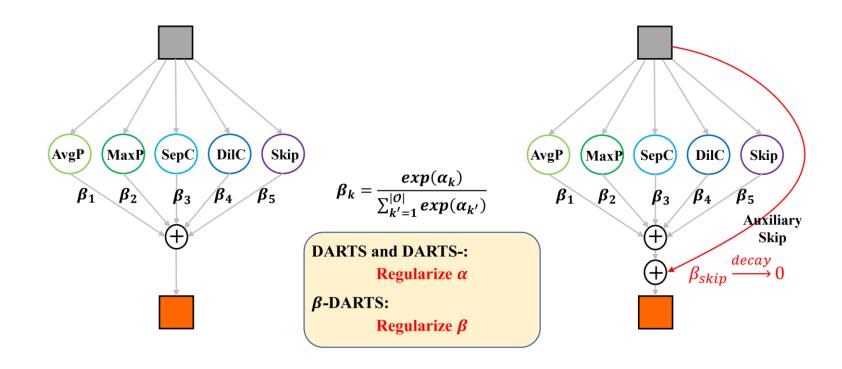
β -DARTS: Beta-Decay Regularization for Differentiable Architecture Search

Peng Ye¹*, Baopu Li², Yikang Li³, Tao Chen¹†, Jiayuan Fan¹, Wanli Ouyang⁴

¹Fudan University, ²BAIDU USA LLC,

³Shanghai AI Laboratory, ⁴The University of Sydney

yepeng20@fudan.edu.cn



Algorithm 1 PyTorch Implementation in DARTS

- 1: $\mathcal{L}_{Beta} = \text{torch.mean(torch.logsumexp(self.model._arch_parameters, dim=-1))}$
- 2: loss = self._val_loss(self.model, input_valid, target_valid)+ $\lambda \mathcal{L}_{Beta}$

Algorithm 2 β -DARTS

Require:

Architecture parameters α ; Network weights w; Number of search epochs E; Regularization coefficient adjustment scheme $\lambda_e, e \in \{1, 2, \dots, E\}$.

- 1: Construct a supernet and initialize architecture parameters α and supernet weights w
- 2: For each $e \in [1, E]$ do
- 3: Update architecture parameters α by descending $\nabla_{\alpha} \mathcal{L}_{val} + \lambda_e \mathcal{L}_{Beta}$
- 4: Update network weights w by descending $\nabla_w \mathcal{L}_{train}$
- 5: Derive the final architecture based on the learned α .

How DARTS update

$$\alpha_k^{t+1} \leftarrow \alpha_k^t - \eta_\alpha \cdot \nabla_{\alpha_k} \mathcal{L}_{val}$$

• Temperature Decay DARTS update

$$\alpha_k^{t+1} \leftarrow \frac{\alpha_k^t - \nabla_{\alpha_k} \mathcal{L}_{val}}{T^{t+1}}$$

Commonly used regularization method on DARTS

$$\bar{\alpha}_{k}^{t+1} \leftarrow \alpha_{k}^{t} - \eta_{\alpha} \cdot \nabla_{\alpha_{k}} \mathcal{L}_{val} - \eta_{\alpha} \lambda \mathcal{N} \left(\alpha_{k}^{t} \right)$$

• What Beta-Decay DARTS suggests

$$\bar{\alpha}_{k}^{t+1} \leftarrow \alpha_{k}^{t} - \eta_{\alpha} \nabla_{\alpha_{k}} \mathcal{L}_{val} - \eta_{\alpha} \lambda F\left(\alpha_{k}^{t}\right)$$

Constrain the value of Beta from changing too much

$$\bar{\beta}_k^{t+1} = \theta_k^{t+1} \left(\alpha_k^t \right) \beta_k^{t+1}$$

Note that,
$$\beta_k^{(i,j)} = \frac{\exp\left(\alpha_k^{(i,j)}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{(i,j)}\right)}$$

Influence of Beta-Decay DARTS

$$\frac{\bar{\beta}_k^{t+1}}{\beta_k^{t+1}} = \frac{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{t+1}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \left[\exp\left(F(\alpha_k^t) - F(\alpha_{k'}^t)\right)\right]^{\lambda \eta_\alpha} \exp\left(\alpha_{k'}^{t+1}\right)}$$

Where,
$$F(\alpha_k) = \frac{\exp(\alpha_k)}{\sum_{k'=1}^{|\mathcal{O}|} \exp(\alpha_{k'})}$$



- The mapping function F has to meet following two points:
 - 1) F is not affected by the amplitude of α
 - To avoid invalid regularization and optimization difficulties
 - 1) F can refplect the relative amplitude of α
 - To impose more penalty on larger amplitude
- So, they have chosen F as

$$F(\alpha_k) = \frac{\exp(\alpha_k)}{\sum_{k'=1}^{|\mathcal{O}|} \exp(\alpha_{k'})}$$

• Therefore,

$$\theta_k^{t+1}\left(\alpha_k^t\right) = \frac{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{t+1}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \left[\exp\left(\frac{\exp(\alpha_k^t) - \exp(\alpha_{k'}^t)}{\sum_{k''=1}^{|\mathcal{O}|} \exp\left(\alpha_{k''}^t\right)}\right)\right]^{\lambda \eta_{\alpha}}} \exp\left(\alpha_{k'}^{t+1}\right)}$$



• And to make the loss function's gradient respective to α equals $F(\alpha)$,

$$\mathcal{L}_{Beta} = \log \left(\sum_{k=1}^{|\mathcal{O}|} e^{\alpha_k} \right) = \operatorname{smoothmax} (\{\alpha_k\})$$

$$\theta_k^{t+1}\left(\alpha_k^t\right) = \frac{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{t+1}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \left[\exp\left(\frac{\exp(\alpha_k^t) - \exp(\alpha_{k'}^t)}{\sum_{k''=1}^{|\mathcal{O}|} \exp\left(\alpha_{k''}^t\right)}\right)\right]^{\lambda \eta_\alpha} \exp\left(\alpha_{k'}^{t+1}\right)}$$

• "As a result, the variance of β is constrained to be smaller, and the value of β is constrained to be closer to its mean, achieving the effect similar to weight decay, thus called Beta-Decay regularization"



Benefit 1) Probability to choose skip connection decreases

- According to theorem revealed by recent work, the convergence of network weights ω can heavily rely on β_{skip} in the supernet.
- Loss can be reduced by ratio $(1 \eta_{\omega} \varphi / 4)$ with probability of at leat 1- σ , where η_{ω} is the corresponding learning rate and will be bounded by σ , and φ obeys.
- 1) Probability to choose skip connection in DARTS

$$\varphi \propto \sum_{i=0}^{h-2} \left[\left(\beta_{conv}^{(i,h-1)} \right)^2 \prod_{t=0}^{i-1} \left(\beta_{skip}^{(t,i)} \right)^2 \right] \quad \text{where,} \quad h \text{ is the number of supernet layers}$$

2) Probability to choose skip connection in Beta-Decay DARTS

$$\varphi \propto \sum_{i=0}^{h-2} \left[\left(\theta_{conv}^{(i,h-1)} \beta_{conv}^{(i,h-1)} \right)^2 \prod_{t=0}^{i-1} \left(\theta_{skip}^{(i,h-1)} \beta_{skip}^{(t,i)} \right)^2 \right]$$

• Note that, θ becomes smaller when β is larger



Benefit 2) Stronger generalization

1. Lipschitz constraint

Let, model = $f_{\omega}(x)$

When $||x_1 - x_2||$ is very small, a well-trained model should meet the following constraints.

$$||f_w(x_1) - f_w(x_2)|| \le C(w) \cdot ||x_1 - x_2||$$

Where, $C(\omega)$ is the Lipschitz constant

• The smaller the constant is, the trained model will be less sensitive to input disturbances and have better generalization ability.



Benefit 2) Stronger generalization

1. Cauchy's inequality

Let,

Operation set: $F_{(x)} = (f_1(x), f_2(x), f_3(x))$

Architecture parameters $\beta = (\beta_1, \beta_2, \beta_3)$

Then, according to Cauchy's inequality,

$$\|\beta F^{T}(x_{1}) - \beta F^{T}(x_{2})\| \leq \|\beta\| \|F^{T}(x_{1}) - F^{T}(x_{2})\|$$

Where,
$$\|\beta\| = \sqrt{\Sigma \beta_i^2}$$
 as Lipschitz constant and, $\Sigma \beta_i = 1$

• As a result, the smaller the measure $\|\beta\|$ is, the supernet will be less sensitive to the impact of input on the operation set, and the searched architecture will have better generalization ability.



Benefit 3) Comparison with commonly-used regularization

1. L2 regularization and weight decay regularization

$$\frac{\bar{\beta}_{k}^{t+1}}{\beta_{k}^{t+1}} = \frac{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{t+1}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \left[\exp\left(\mathcal{N}(\alpha_{k}^{t}) - \mathcal{N}(\alpha_{k'}^{t})\right)\right]^{\lambda \eta_{\alpha}} \exp\left(\alpha_{k'}^{t+1}\right)}$$

- When values in α are all around one, regularization has little effect on Beta.
- When the median of α is equal to 0, has the same effect with Beta regularization.
- Large variance of α makes optimization process more sensitive to the hyperparameter λ and η_{α} .



Benefit 3) Comparison with commonly-used regularization

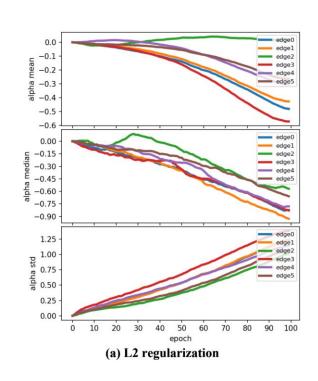
2. Beta-Decay regularization

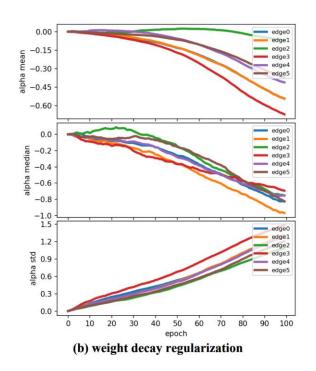
$$\frac{\bar{\beta}_{k}^{t+1}}{\beta_{k}^{t+1}} = \frac{\sum_{k'=1}^{|\mathcal{O}|} \exp\left(\alpha_{k'}^{t+1}\right)}{\sum_{k'=1}^{|\mathcal{O}|} \left[\exp\left(\alpha_{k}^{t} - \alpha_{k'}^{t}\right)\right]^{\lambda \eta_{\alpha}} \exp\left(\alpha_{k'}^{t+1}\right)}$$

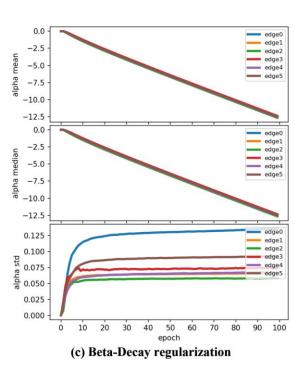
- The mean and median of α are basically equal.
- When the standard deviation of α increases to a certain extent, it will remain unchanged.



Benefit 3) Comparison with commonly-used regularization







 Search on NAS-Bench-201 CIFAR-10 dataset, Adapt on NAS-Bench-201 CIFAR-10, NAS-Bench-201 CIFAR-100, NAS-Bench-201 ImageNet16-120

Table 1. Performance comparison on NAS-Bench-201 benchmark [9]. Note that β -DARTS only searches on CIFAR-10 dataset, but can robustly achieve new SOTA on CIFAR-10, CIFAR-100 and ImageNet16-120. Averaged on 4 independent runs of searching.

Methods	Cost	CIFA	R-10	CIFA	R-100	ImageNet16-120		
Methous	(hours)	valid	test	valid	test	valid	test	
DARTS(1st) [21]	3.2	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00	
DARTS(2nd) [21]	10.2	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00	
GDAS [8]	8.7	89.89±0.08	93.61±0.09	71.34±0.04	70.70 ± 0.30	41.59±1.33	41.71±0.98	
SNAS [28]	-	90.10±1.04	92.77±0.83	69.69±2.39	69.34±1.98	42.84±1.79	43.16±2.64	
DSNAS [16]	-	89.66±0.29	93.08±0.13	30.87 ± 16.40	31.01±16.38	40.61±0.09	41.07±0.09	
PC-DARTS [29]	-	89.96±0.15	93.41±0.30	67.12±0.39	67.48±0.89	40.83±0.08	41.31±0.22	
iDARTS [31]	-	89.86±0.60	93.58±0.32	70.57±0.24	70.83±0.48	40.38±0.59	40.89±0.68	
DARTS- [5]	3.2	91.03±0.44	93.80±0.40	71.36±1.51	71.53±1.51	44.87±1.46	45.12±0.82	
$\beta ext{-DARTS}$	3.2	91.55±0.00	94.36±0.00	73.49 ± 0.00	73.51±0.00	46.37 ± 0.00	46.34±0.00	
optimal	-	91.61	94.37	73.49	73.51	46.77	47.31	

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PC-DARTS [29]	-	89.96±0.15	93.41±0.30	67.12±0.39	67.48±0.89	40.83±0.08	41.31±0.22	
iDARTS [31]	-	89.86±0.60	93.58±0.32	70.57±0.24	70.83±0.48	40.38±0.59	40.89±0.68	
DARTS- [5]	3.2	91.03±0.44	93.80±0.40	71.36±1.51	71.53±1.51	44.87±1.46	45.12±0.82	
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optimal	-	91.61	94.37	73.49	73.51	46.77	47.31	



- ++ : Search on CIFAR-100, test on CIFAR-10 and CIFAR-100
- +: Search on CIFAR-10, test on CIFAR-10 and CIFAR-100
- Search on ImageNet / Cross Domain(CIFAR-10 and part of ImageNet) / CIFAR-10 or CIFAR-100

Method	GPU	CIFA	AR-10	CIFAR-100		Method	GPU	Params	FLOPs	Top1	Top5
Method	(Days) $\overline{\text{Params}(M)}$ $\overline{\text{Acc}(\%)}$ $\overline{\text{Params}(M)}$ $\overline{\text{Acc}(\%)}$		Wethod	(Days)	(M)	(\mathbf{M})	(%)	(%)			
NASNet-A [33]	2000	3.3	97.35	3.3	83.18	MnasNet-92*(Img.) [26]	1667	4.4	388	74.8	92.0
DARTS(1st) [21]	0.4	3.4	97.00±0.14	3.4	82.46	FairDARTS*(Img.) [6]	3	4.3	440	75.6	92.6
DARTS(2nd) [21]	1	3.3	97.24±0.09	-	-	PC-DARTS(Img.) [29]	3.8	5.3	597	75.8	92.7
SNAS [28]	1.5	2.8	97.15±0.02	2.8	82.45	DOTS(Img.) [12]	1.3	5.3	596	76.0	92.8
GDAS [8]	0.2	3.4	97.07	3.4	81.62	DARTS-*(Img.) [5]	4.5	4.9	467	76.2	93.0
P-DARTS [4]	0.3	3.4	97.50	3.6	82.51	AdaptNAS-S(CD.) [19]	1.8	5.0	552	74.7	92.2
PC-DARTS [29]	0.1	3.6	97.43±0.07	3.6	83.10	AdaptNAS-C(CD.) [19]	2.0	5.3	583	75.8	92.6
P-DARTS [4]	0.3	3.3±0.21	97.19±0.14	-	-	AmoebaNet-C(C10) [25]	3150	6.4	570	75.7	92.4
R-DARTS(L2) [1]	1.6	-	97.05±0.21	-	81.99±0.26	SNAS(C10) [28]	1.5	4.3	522	72.7	90.8
SDARTS-ADV [3]	1.3	3.3	97.39±0.02	-	-	P-DARTS(C100) [4]	0.3	5.1	577	75.3	92.5
DOTS [12]	0.3	3.5	97.51±0.06	4.1	83.52±0.13	SDARTS-ADV(C10) [3]	1.3	5.4	594	74.8	92.2
DARTS+PT [27]	0.8	3.0	97.39±0.08	-	-	DOTS(C10) [12]	0.3	5.2	581	75.7	92.6
DARTS- [5]	0.4	3.5 ± 0.13	97.41±0.08	3.4	82.49±0.25	DARTS+PT(C10) [27]	0.8	4.6	-	74.5	92.0
β -DARTS ‡	0.4	3.78 ± 0.08	97.49±0.07	3.83 ± 0.08	83.48±0.03	β -DARTS(C100)	0.4	5.4	597	75.8	92.9
β -DARTS [†]	0.4	3.75±0.15	97.47±0.08	3.80±0.15	83.76±0.22	β -DARTS(C10)	0.4	5.5	609	76.1	93.0

• Search on Different Weighting Scheme (Increase)

Table 3. Influence of different weighting schemes on β -DARTS.

Weighting Scheme	CIFAR-10 valid	CIFAR-10 test
0-15/25/50/100	91.21/91.55/91.55/91.55	93.83/94.36/94.36/94.36
5/10/15/25	84.96/90.59/91.55/90.59	88.02/93.31/94.36/93.31
25-15/10/5/0	90.59/87.30/73.58/39.77	93.31/90.65/76.88/54.30

• Comparison of different weighting schemes

Table 4. The results of different Beta regularization loss with different weighting schemes on NAS-Bench-201 benchmark. Note that we only search on CIFAR-10 dataset, and perform 2 runs of searching under different random seeds.

Methods	Weighting CIFAR-10			CIFA	R-100	ImageNet16-120		
	Scheme	valid	test	valid	test	valid	test	
DARTS(1st) [21]	3.2	39.77±0.00	54.30±0.00	15.03±0.00	15.61±0.00	16.43±0.00	16.32±0.00	
Beta-Global	0-25	91.55/91.55	94.36/94.36	73.49/73.49	73.51/73.51	46.37/46.37	46.34/46.34	
Beta-Global	0-50	91.55/91.55	94.36/94.36	73.49/73.49	73.51/73.51	46.37/46.37	46.34/46.34	
Beta-Global	0-75	91.55/91.55	94.36/94.36	73.49/73.49	73.51/73.51	46.37/46.37	46.34/46.34	
Beta-Global	0-100	91.21/91.55	93.83/94.36	71.60/73.49	71.88/73.51	45.75/46.37	44.65/46.34	
Beta-Zero	0-25	91.21/90.97	93.83/93.91	71.60/70.41	71.88/70.78	45.75/43.77	44.65/44.78	
Beta-Zero	0-50	91.55/91.21	94.36/93.83	73.49/71.60	73.51/71.88	46.37/45.74	46.34/44.65	
Beta-Zero	0-75	91.61/91.05	94.37/93.66	72.75/71.02	73.22/71.38	45.56/45.23	46.71/44.70	
Beta-Zero	0-100	91.21/91.21	93.83/93.83	71.60/71.60	71.88/71.88	45.75/45.75	44.65/44.65	



- 1. Change the Loss function
 - Examples from Beta-Decay DARTS paper

$$\mathcal{L}_{Beta-Global} = \operatorname{smoothmax} \left(\alpha_1^1, \cdots, \alpha_{|\mathcal{O}|}^L \right)$$
$$= \log \left(\sum_{l=1}^L \sum_{k=1}^{|\mathcal{O}|} e^{\alpha_k^l} \right)$$

$$\mathcal{L}_{Beta-Zero} = \operatorname{smoothmax} \left(0, \alpha_k^l \right)$$
$$= -\log \left(1 + e^{-\alpha_k^l} \right)$$

- 2. Use different Weighting Scheme
- 3. Make θ as learnable parameter



- DARTS: Differentiable Architecture Search https://arxiv.org/abs/1806.09055
- β-DARTS: Beta-Decay Regularization for Differentiable Architecture Search https://arxiv.org/abs/2203.01665
- Theory-Inspired Path-Regularized Differential Network Architecture Search https://arxiv.org/abs/2006.16537



Thank you Q & A