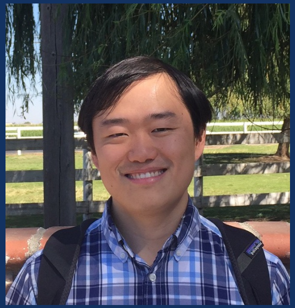
Understanding self-supervised Learning Dynamics without Contrastive Pairs



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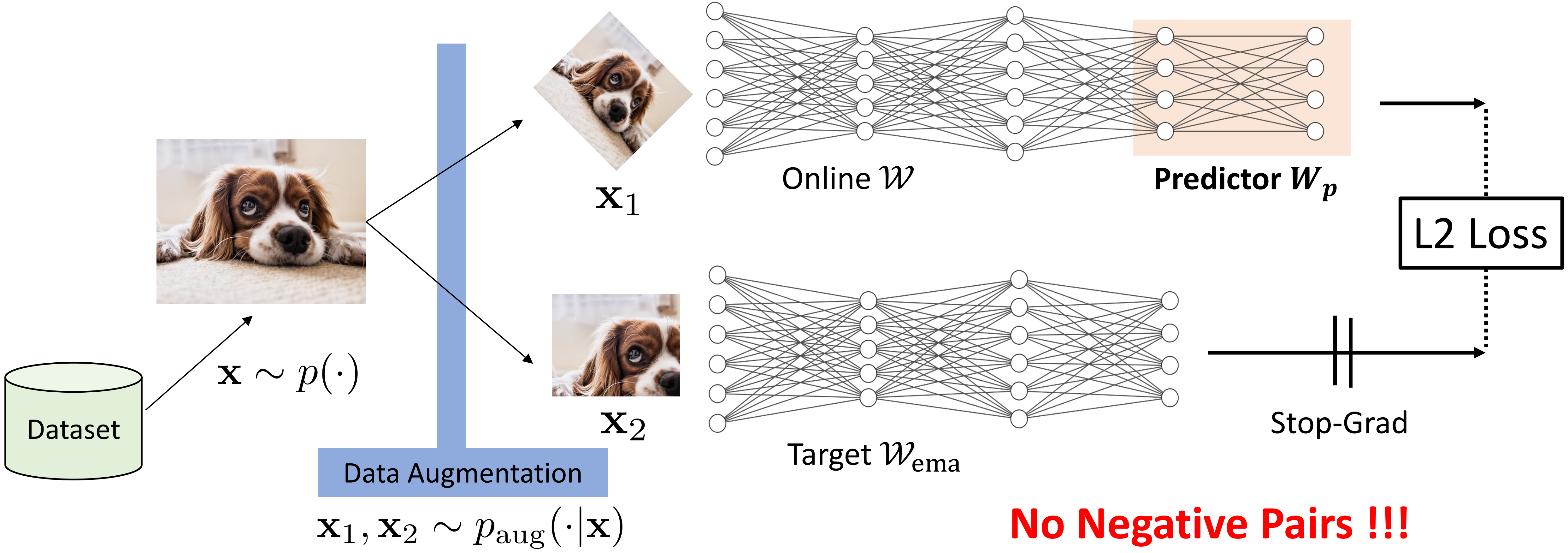
ICML 2021

Code: https://github.com/facebookresearch/luckmatters/tree/master/ssl

facebook Artificial Intelligence

Non-contrastive SSL (BYOL/SimSiam)

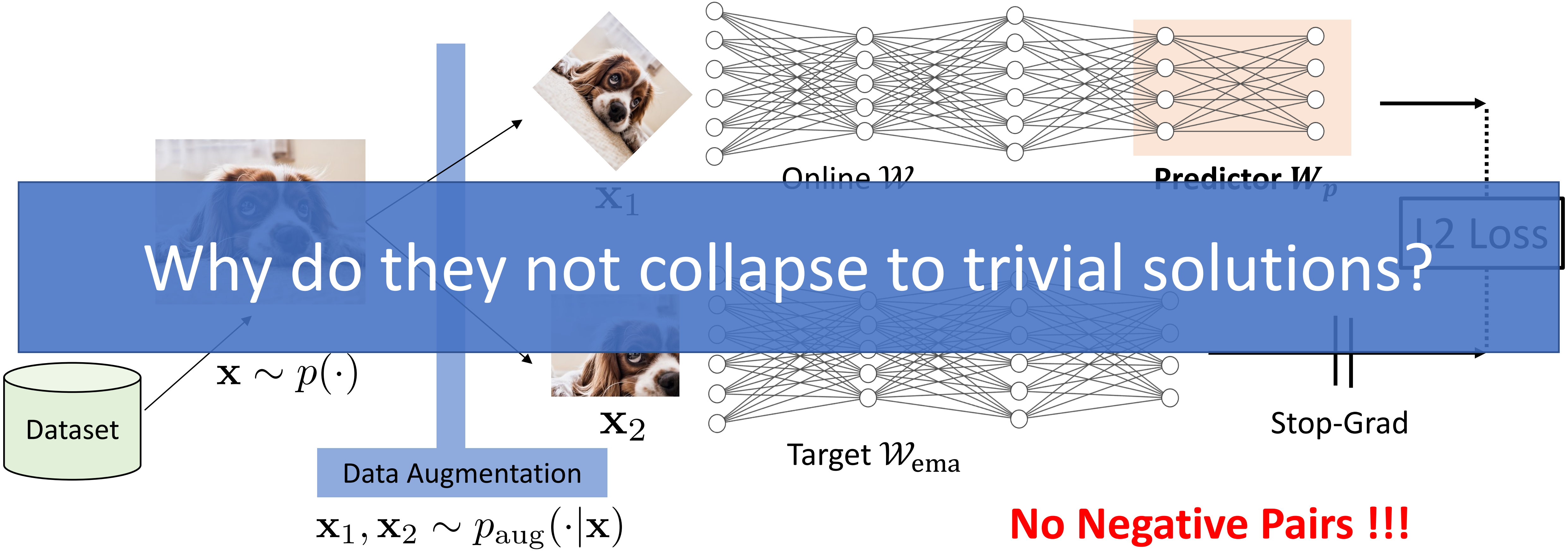


No Negative Pairs !!!

BYOL: *[J. Grill, Bootstrap your own latent: A new approach to self-supervised Learning, NeurIPS 2020]*

SimSiam: *[X. Chen and K. He, Exploring Simple Siamese Representation Learning, CVPR 2021]*

Non-contrastive SSL (BYOL/SimSiam)?



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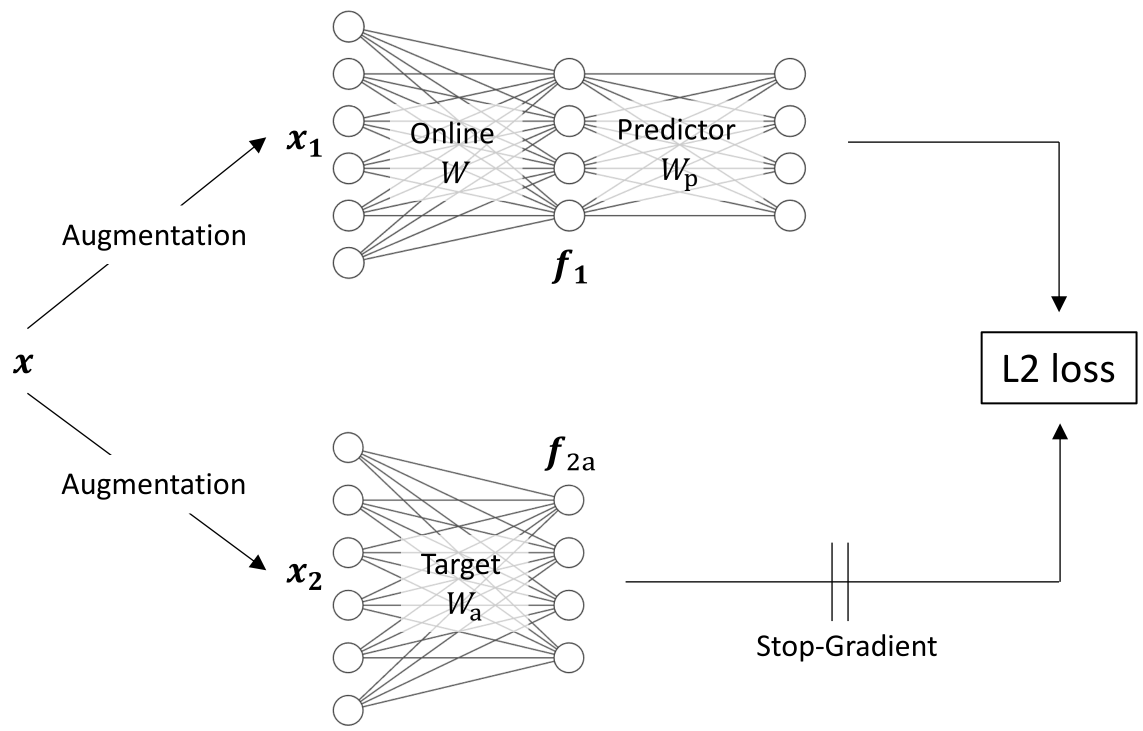
A simple model



Objective:

$$J(W, W_p) := \frac{1}{2}\mathbb{E}_{\boldsymbol{x}_1,\boldsymbol{x}_2}\left[\|W_p \boldsymbol{f}_1 - \mathrm{StopGrad}(\boldsymbol{f}_{2\mathrm{a}})\|_2^2\right]$$

Linear online network W

Linear target network W_a

Linear predictor W_p

The Dynamics of Training Procedure

Lemma 1. *BYOL learning dynamics following Eqn. 1:*

$$\dot{W}_p = \alpha_p \left(-W_p W (X + X') + W_\mathrm{a} X\right) W^\intercal - \eta W_p$$
$$\dot{W} = W_p^\intercal \left(-W_p W (X + X') + W_\mathrm{a} X\right) - \eta W$$
$$\dot{W}_\mathrm{a} = \beta(-W_\mathrm{a} + W)$$

$$\bar{\boldsymbol{x}}(\boldsymbol{x}) := \mathbb{E}_{\boldsymbol{x}' \sim p_\mathrm{aug}(\cdot|\boldsymbol{x})}\left[\boldsymbol{x}'\right]$$

$X = \mathbb{E}\left[\bar{\boldsymbol{x}}\bar{\boldsymbol{x}}^\intercal\right]$ Covariance of the data

$X' = \mathbb{E}_{\boldsymbol{x}}\left[\mathbb{V}_{\boldsymbol{x}'|\boldsymbol{x}}[\boldsymbol{x}']\right]$ Covariance of the augmentation

Part I Why we need (1) an **extra predictor** and (2) **stop-gradient**?

Part II Why the system doesn't **collapse** to trivial solutions?

Part III The role played by different hyperparameters

Hyperparameter	Description
α_p	Relative learning rate of the predictor
η	Weight decay
β	The rate of Exponential Moving Average (EMA)

Part IV Novel non-contrastive SSL algorithm **DirectPred**

Part I No Predictor / No Stop-Gradient do not work

If there is no EMA ($W = W_a$), then the dynamics changes:

No Predictor

$$\dot{W} = -\underbrace{(X' + \eta I)}_{\text{PSD matrix}}W$$

No Stop-Gradient (Here $\widetilde{W_p} := W_p - I$)

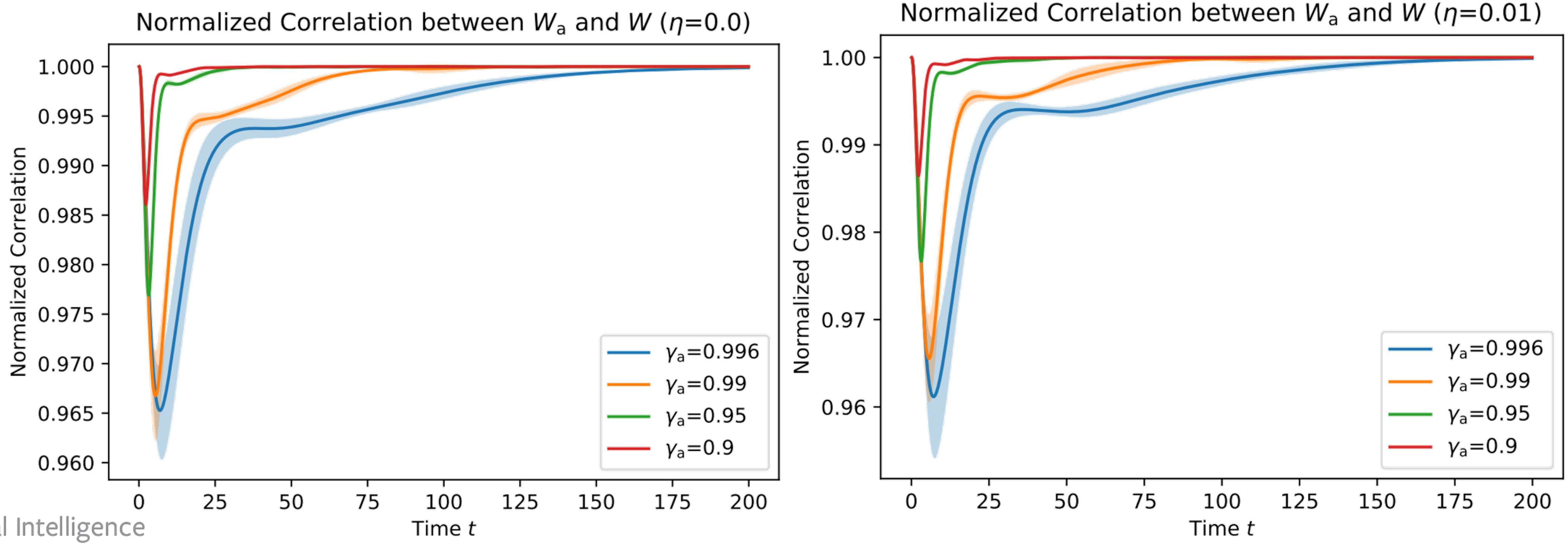
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{vec}(W) = -\underbrace{\left[X' \otimes (W_p^\intercal W_p + I) + X \otimes \tilde{W}_p^\intercal \tilde{W}_p + \eta I_{n_1 n_2}\right]}_{\text{PSD matrix}} \mathrm{vec}(W)$$

In both cases, $W \to 0$

Part II Assumptions

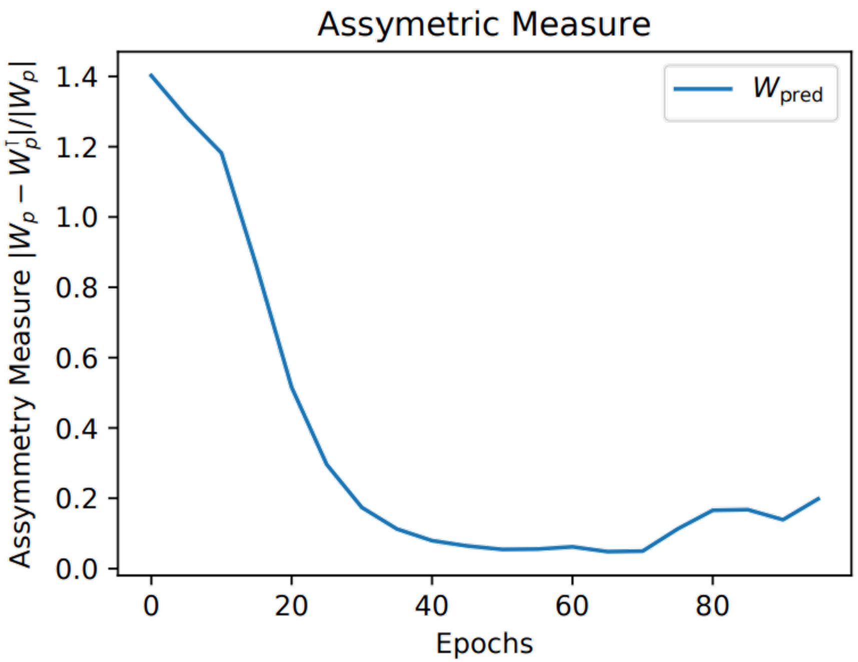
Assumption 1 (Isotropic Data and Augmentation): $X = I$ and $X' = \sigma^2 I$

Assumption 2: the EMA weight $W_a(t) = \tau(t)W(t)$ is a linear function of $W(t)$



Symmetrization of the dynamics

<u>*Assumption 3*</u> (Symmetric predictor W_p): $W_p(t) = W_p^T(t)$



W_p becomes increasingly symmetric over training

	No predictor bias sym W_p	No predictor bias regular W_p	With predictor bias sym W_p	With predictor bias regular W_p
One-layer linear predictor				
EMA	75.09 ± 0.48	74.51 ± 0.47	74.52 ± 0.29	74.16 ± 0.33
no EMA	**36.62 ± 1.85**	72.85 ± 0.16	**36.04 ± 2.74**	72.13 ± 0.53
Two-layer predictor with BatchNorm and ReLU				
EMA	71.58 ± 6.46	78.85 ± 0.25	77.64 ± 0.41	78.53 ± 0.34
no EMA	**35.59 ± 2.10**	65.98 ± 0.71	**41.92 ± 4.25**	65.59 ± 0.66

Perfect symmetric W_p might hurt training

Symmetrized Dynamics

Under the three assumptions, the dynamics becomes:

$$
\begin{aligned}
\dot{W}_p &= -\frac{\alpha_p}{2}(1+\sigma^2)\{W_p, F\} + \alpha_p \tau F - \eta W_p \\
\dot{F} &= -(1+\sigma^2)\{W_p^2, F\} + \tau\{W_p, F\} - 2\eta F
\end{aligned}
$$

$\{A, B\} \coloneqq AB + BA$ is the anti-commutator.

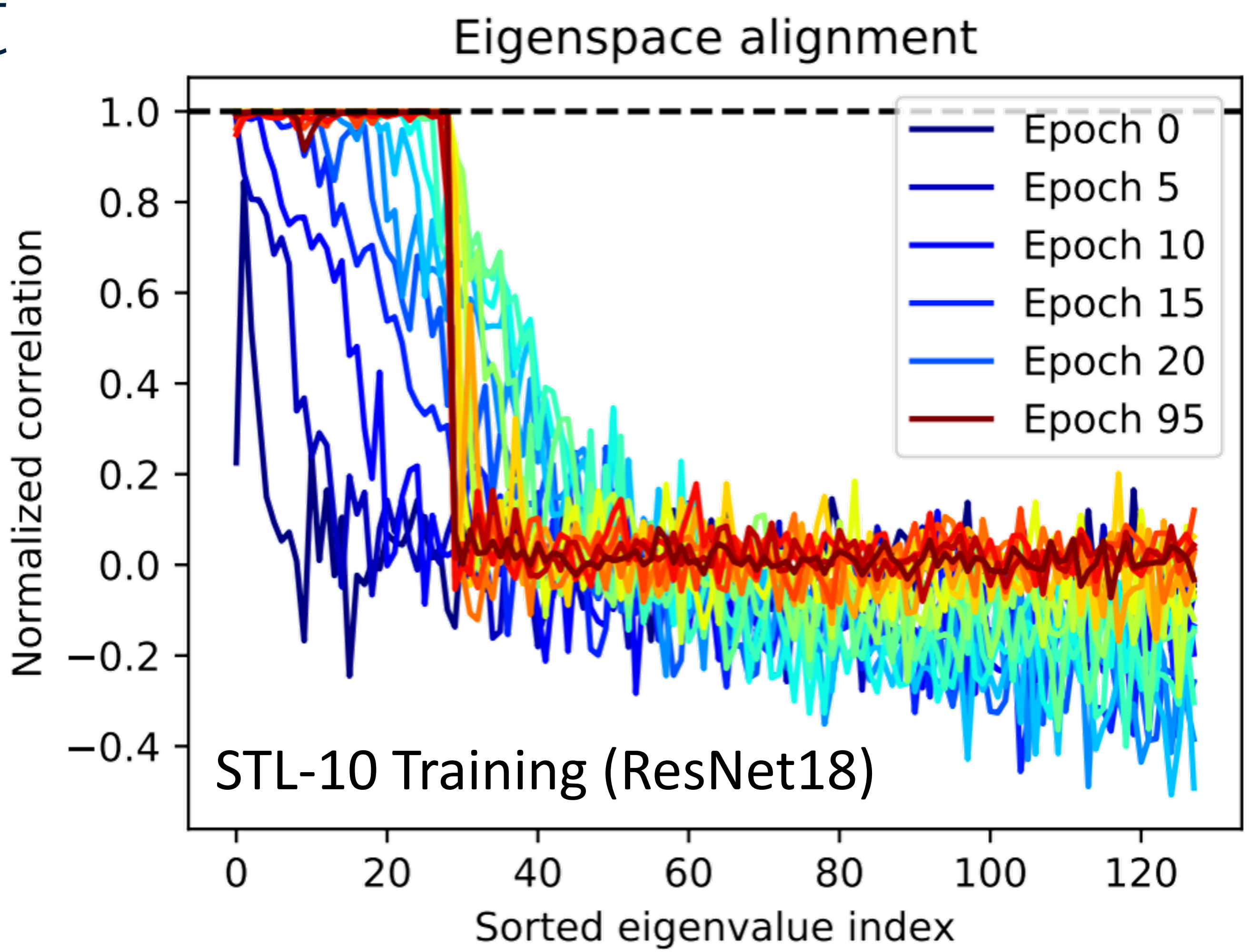
Here $F \coloneqq \mathrm{E}[ff^T] = WXW^T$ is the correlation matrix of the input of the predictor W_p. F is well-defined even with nonlinear network.

Eigenspace Alignment

Theorem 3: Under certain conditions,

$$FW_p - W_pF \to 0$$

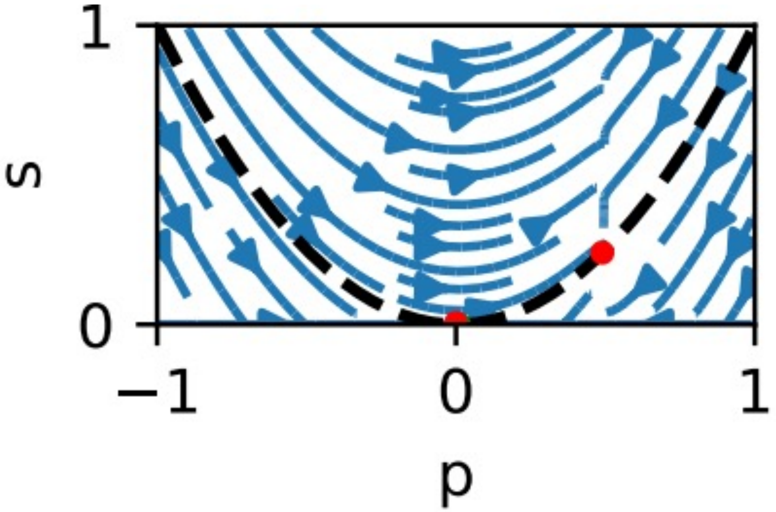
and the eigenspace of W_p and F gradually **aligns**.



Why non-contrastive SSL doesn't collapse?

When eigenspace aligns, the dynamics becomes decoupled:

$$\begin{aligned}\dot{p}_j &= \alpha_p s_j \left[\tau - (1+\sigma^2)p_j\right] - \eta p_j \\ \dot{s}_j &= 2p_j s_j \left[\tau - (1+\sigma^2)p_j\right] - 2\eta s_j \\ s_j\dot{\tau} &= \beta(1-\tau)s_j - \tau\dot{s}_j/2.\end{aligned}$$



Where p_j and s_j are eigenvalues of W_p and F

Invariance holds: $s_j(t) = \alpha_p^{-1}p_j^2(t) + e^{-2\eta t}c_j$

Why non-contrastive SSL doesn't collapse?

1D dynamics of the eigenvalue p_j of W_p:

$$\dot{p}_j = p_j^2 \left[\underbrace{\tau(t)}_{\text{EMA}} - (1 + \underbrace{\sigma^2}_{\text{Variance due to data augmentation}})p_j\right] - \underbrace{\eta}_{\text{Weight Decay}} p_j$$

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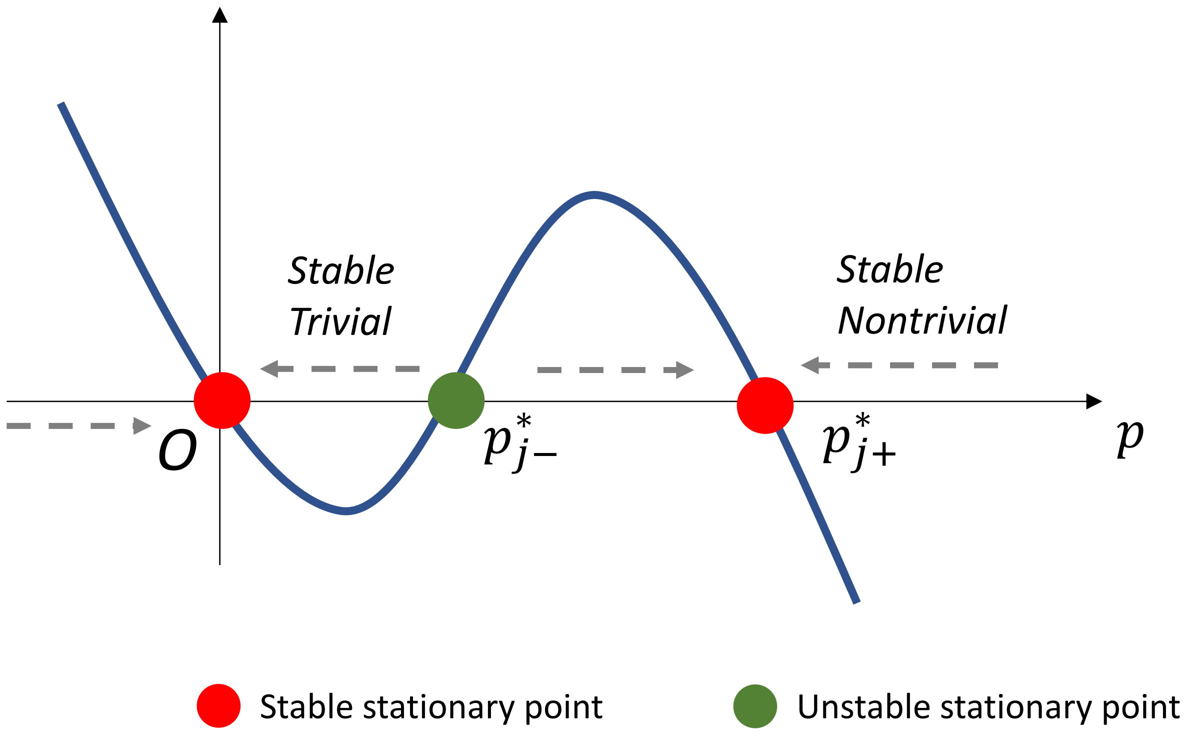

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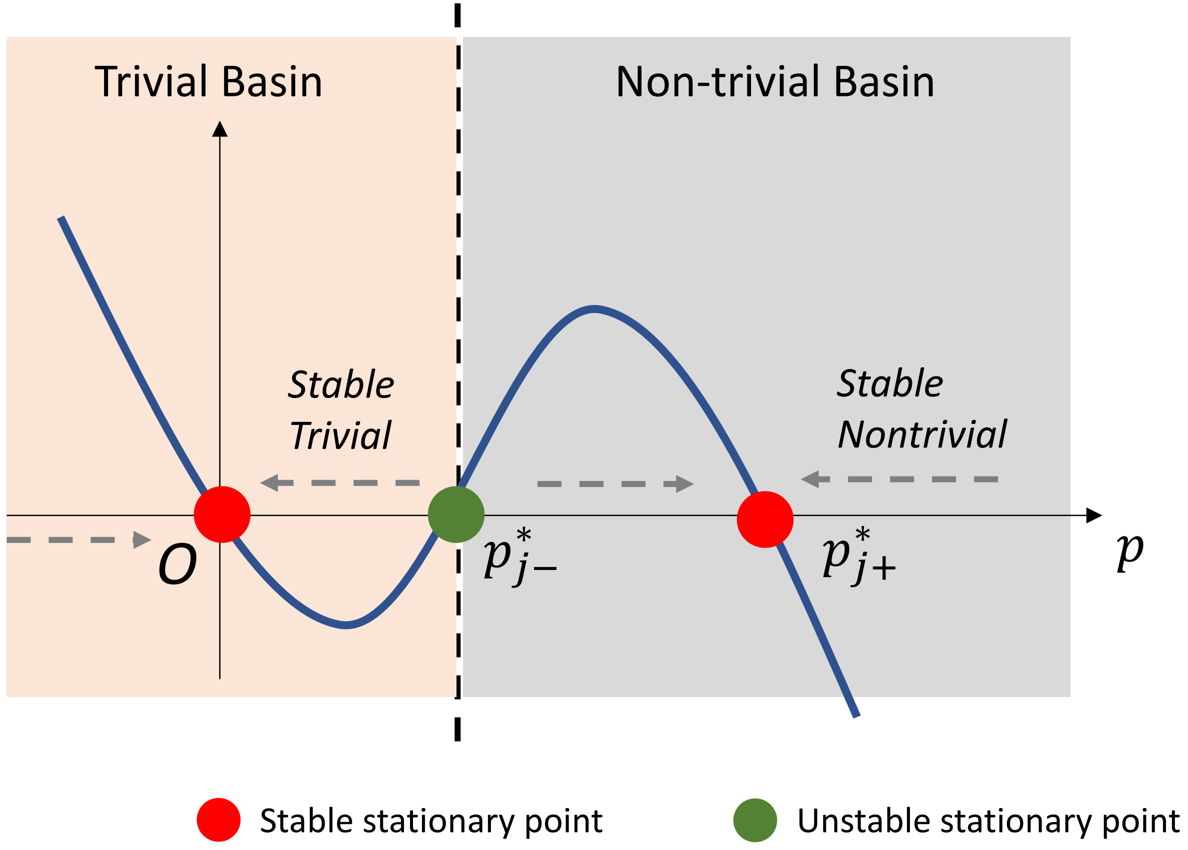
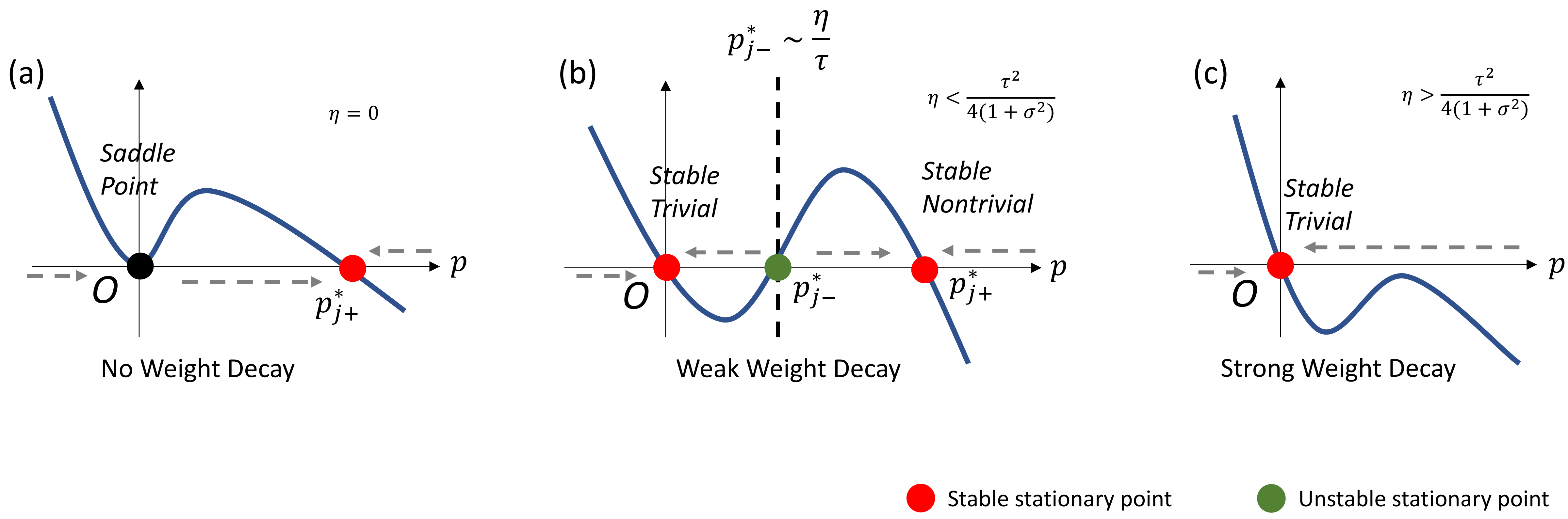
$$p^*_{j-} = \frac{\tau - \sqrt{\tau^2 - 4\eta(1+\sigma^2)}}{2(1+\sigma^2)} \sim \frac{\eta}{\tau}$$



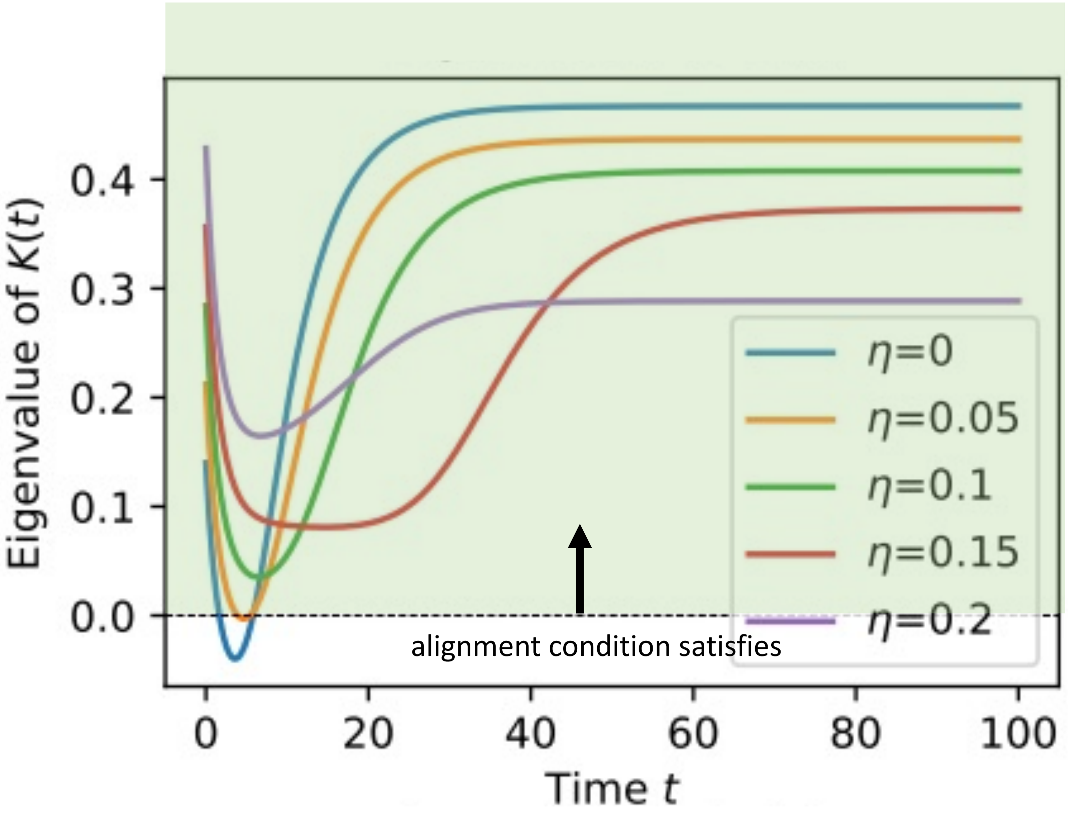
Part III The Effect of Weight Decay η



The Benefit of Weight Decay

Eigenspace alignment condition

$$p_j[\tau - (1+\sigma^2)p_j] < \frac{1}{2}[\alpha_p(1+\sigma^2)s_j + 3\eta]$$

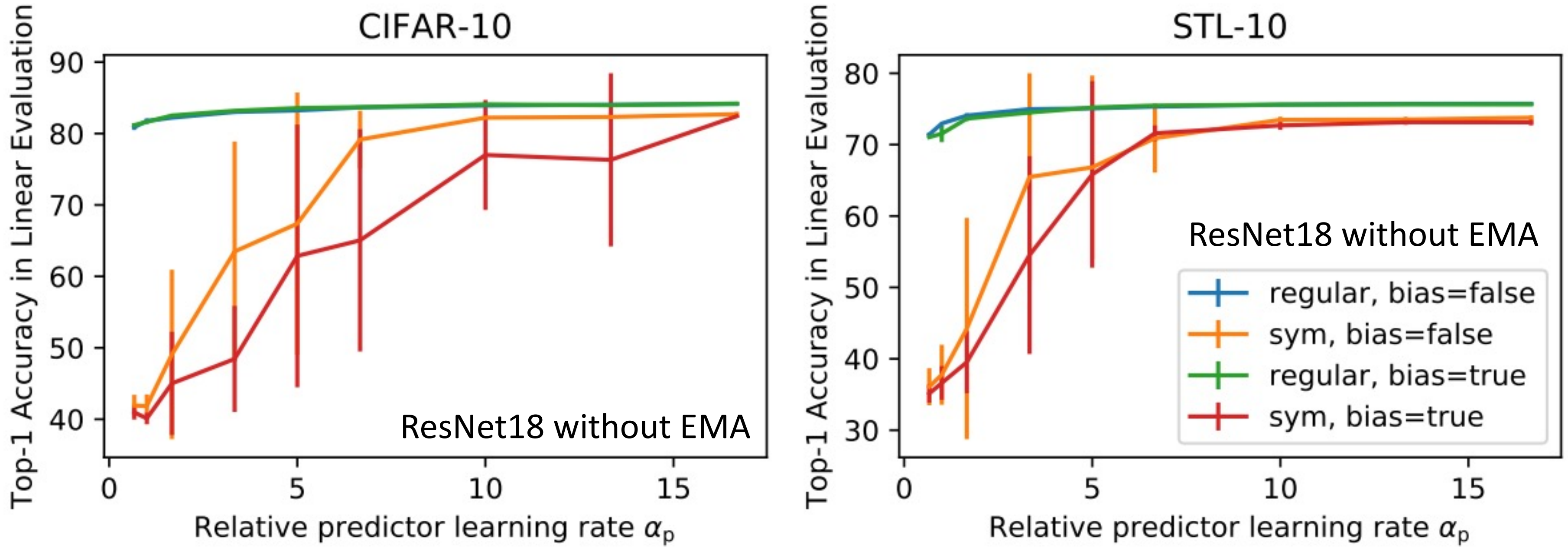


Higher weight decay → alignment condition is more likely to satisfy!

Relative learning rate of the predictor $\boldsymbol{\alpha_p}$

Positive ☺

1. Large α_p shrinks the size of trivial basin
2. Relax the condition of eigenspace alignment



Negative ☹ With very large α_p, eigenvalue of F won't grow (and no feature learning)

Exponential Moving Average rate $\boldsymbol{\beta}$

β large → $W_a(t)$ catches $W(t)$ faster → τ grows faster to 1

Positive ☺: Slower rate (small β) relaxes the condition of eigenspace alignment

Negative ☹: Slower rate makes the training slow and expands the size of trivial basin

Part IV DirectPred

- Directly setting linear W_p rather than relying on gradient update.

1. Estimate $\hat{F} = \rho\hat{F} + (1-\rho)E[\boldsymbol{f}\boldsymbol{f}^T]$
2. Eigen-decompose $\hat{F} = \hat{U}\Lambda_F\hat{U}^T$, $\Lambda_F = \mathrm{diag}\,[s_1, s_2, \ldots, s_d]$
3. Set W_p following the invariance:

$$p_j = \sqrt{s_j} + \epsilon \max_j s_j, \quad W_p = \hat{U}\mathrm{diag}[p_j]\hat{U}^\intercal$$

Guaranteed Eigenspace Alignment ☺

Performance of **DirectPred** on STL-10/CIFAR-10

Downstream Classification Top-1	Number of epochs 100	300	500
STL-10			
DirectPred	$\mathbf{77.86 \pm 0.16}$	78.77 ± 0.97	78.86 ± 1.15
DirectPred (freq=5)	77.54 ± 0.11	$\mathbf{79.90 \pm 0.66}$	$\mathbf{80.28 \pm 0.62}$
SGD baseline	75.06 ± 0.52	75.25 ± 0.74	75.25 ± 0.74
CIFAR-10			
DirectPred	$\mathbf{85.21 \pm 0.23}$	$\mathbf{88.88 \pm 0.15}$	89.52 ± 0.04
DirectPred (freq=5)	84.93 ± 0.29	88.83 ± 0.10	$\mathbf{89.56 \pm 0.13}$
SGD baseline	84.49 ± 0.20	88.57 ± 0.15	89.33 ± 0.27

Performance of **DirectPred** on ImageNet

Downstream classification (ImageNet):

BYOL variants	*Accuracy (60 ep)*		*Accuracy (300 ep)*	
	Top-1	Top-5	Top-1	Top-5
2-layer predictor*	**64.7**	**85.8**	**72.5**	90.8
linear predictor	59.4	82.3	69.9	89.6
DirectPred	64.4	**85.8**	72.4	**91.0**

* 2-layer predictor is BYOL default setting.

DirectPred using linear predictor is better than SGD with linear predictor, and is comparable with 2-layer predictor.

Conclusion

- A systematic analysis on the dynamics of non-contrastive self-supervised learning (SSL) methods
  - **Part I** Why we need (1) an **extra predictor** and (2) **stop-gradient**?
  - **Part II** Why training doesn't **collapse** to trivial solutions?
  - **Part III** The role played by different hyperparameters
- Propose **DirectPred**, a novel non-contrastive SSL method
  - Directly align the eigenspace of the predictor W_p with the correlation matrix F
  - Comparable performance in downstream classification tasks, compared to vanilla BYOL
    - CIFAR-10/STL-10
    - ImageNet (60 epochs / 300 epochs)

Code: https://github.com/facebookresearch/luckmatters/tree/master/ssl

Thanks!