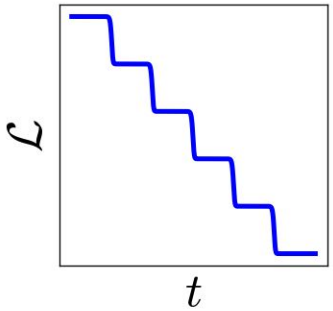
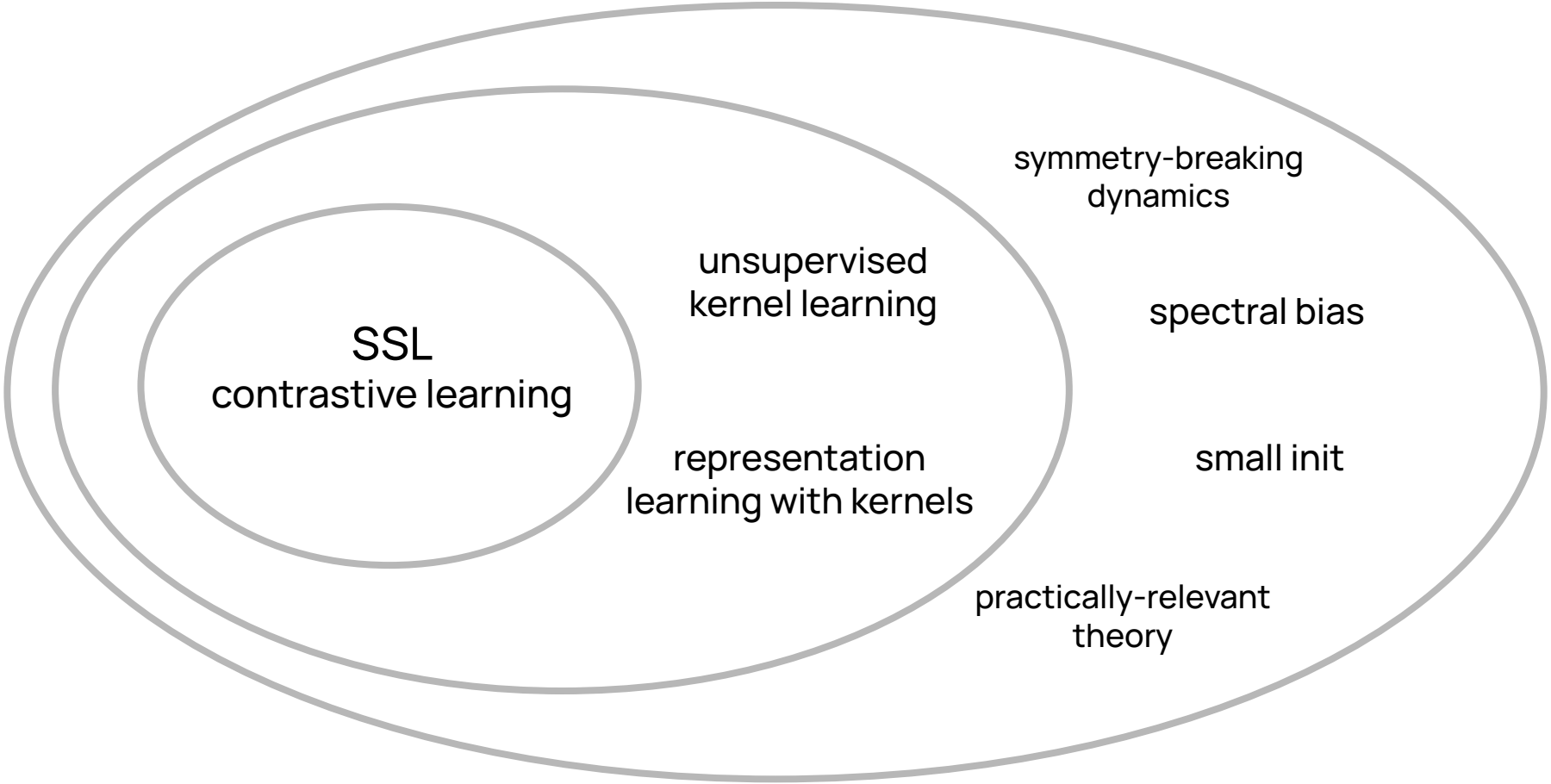
On the stepwise nature of SSL



Jamie Simon

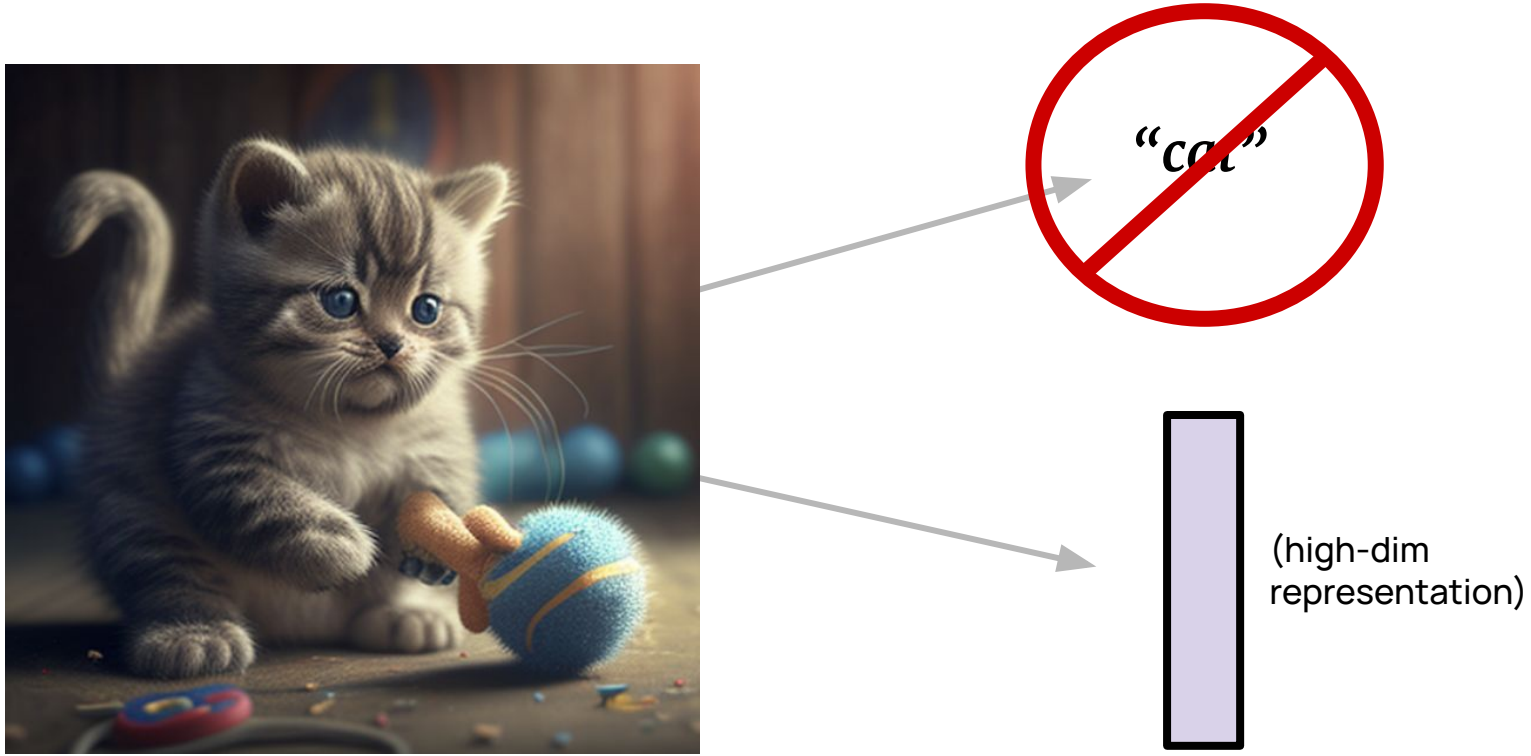
with Maksis Knutins, Liu Ziyin, Daniel Geisz, Abe Fetterman, and Josh Albrecht

paper: tinyurl.com/stepwise-ssl-paper

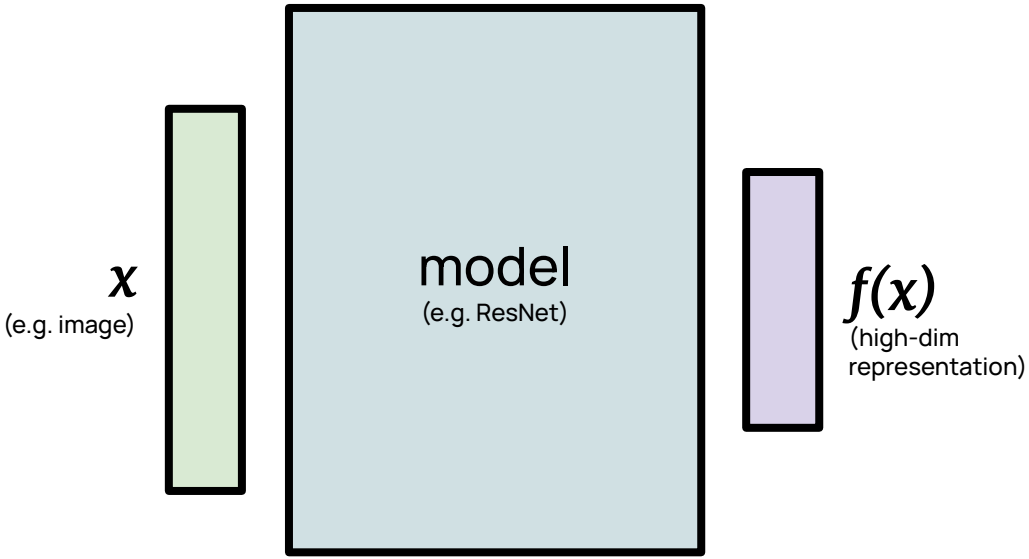

symmetry-breaking
dynamics
unsupervised
kernel learning
spectral bias
SSL
contrastive learning
representation
learning with kernels
small init
practically-relevant
theory

As theorists, we ought to look beyond supervised learning.

We should think about learning *representations*, not *target functions*.



Joint embedding SSL learns representations with a simple prescription.



let x, x' be two related samples.

goal of training: **make $f(x)$ close to $f(x')$**

(but not degenerate)

Surprisingly, this works very well…

SimCLR, Barlow Twins, VICReg, BYOL, DINO, CLIP

A Simple Framework for Contrastive Learning of Visual Representations

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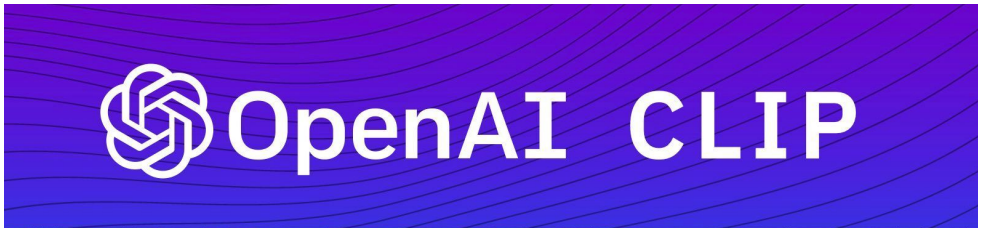
Ting Chen [1] Simon Kornblith [1] Mohammad Norouzi [1] Geoffrey Hinton [1]



SSL is state-of-the-art in image domains.

…but here’s what we understand about it:

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What is the nature of the learning process of SSL?

What representations are ultimately learned?

Idea: answer these Qs in the linear case and check agreement with deep nets.

Plan of attack

1. Find and solve an exactly solvable case of SSL with a **linear model.**
2. Kernelize it.
3. Check agreement with realistic SSL.

Linear model of **Barlow Twins** (Zbontar et al. 2021)

Let the dataset contain n "positive pairs" $(\mathbf{x}_i, \mathbf{x}'_i)_{i=1}^n$.

Let the trained function be linear as $\mathbf{f}(\mathbf{x}) = \mathbf{W}\mathbf{x}$.

Correlation matrix: $\boldsymbol{C} \equiv \frac{1}{2n} \sum_i \left(\boldsymbol{f}(\boldsymbol{x}_i) \boldsymbol{f}(\boldsymbol{x}'_i)^\top + \boldsymbol{f}(\boldsymbol{x}'_i) \boldsymbol{f}(\boldsymbol{x}_i)^\top \right)$

Barlow Twins loss: $\mathcal{L} = \|\boldsymbol{C} - \boldsymbol{I}_d\|_F^2$

Train with GD: $\frac{d\boldsymbol{W}}{dt} = -\nabla_{\boldsymbol{W}} \mathcal{L}.$

Key insight: diagonalize w.r.t. the “feature cross-covariance.”

$$\boldsymbol{\Gamma} \equiv \frac{1}{2n} \sum_i \left(\boldsymbol{x}_i \boldsymbol{x}_i'^\top + \boldsymbol{x}_i' \boldsymbol{x}_i^\top \right)$$

$$\Longrightarrow \qquad \mathcal{L} = \left\| \boldsymbol{W} \boldsymbol{\Gamma} \boldsymbol{W}^\top - \boldsymbol{I}_d \right\|_F^2$$

$$\Longrightarrow \qquad \frac{d\boldsymbol{W}}{dt} = -4 \left(\boldsymbol{W} \boldsymbol{\Gamma} \boldsymbol{W}^\top - \boldsymbol{I}_d \right) \boldsymbol{W} \boldsymbol{\Gamma}$$

^This is *exactly solvable* when $\boldsymbol{W_o}$ = $\boldsymbol{W(t=o)}$ is either *aligned* or *small*.

Aligned init: $\boldsymbol{W}_0 = \boldsymbol{U} \boldsymbol{S}_0 \boldsymbol{\Gamma}^{(\leq d)}$

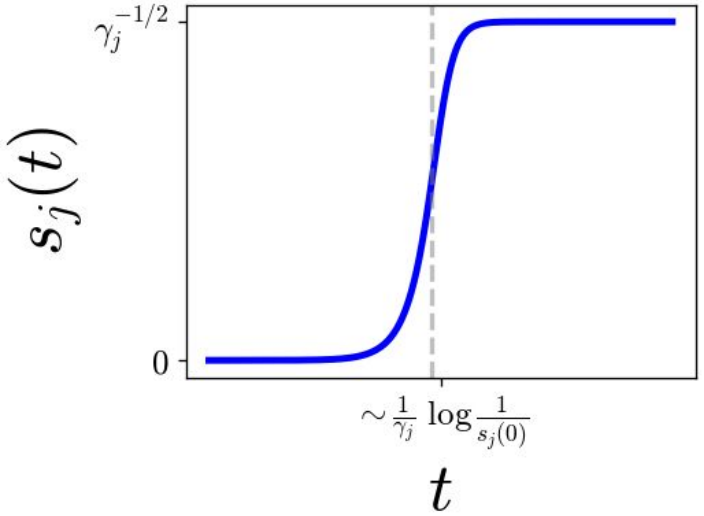
right singular vectors are
the top d eigenvectors of $\boldsymbol{\Gamma}$

From aligned init, each singular value evolves independently.

Proposition 4.1 (Trajectory of $\boldsymbol{W}(t)$ from aligned initialization). *If $\boldsymbol{W}(0) = \boldsymbol{W}_0$ as given by Equations 7 and 8, then*

$$\boldsymbol{W}(t) = \boldsymbol{U}\boldsymbol{S}(t)\boldsymbol{\Gamma}^{(\leq d)} \tag{9}$$

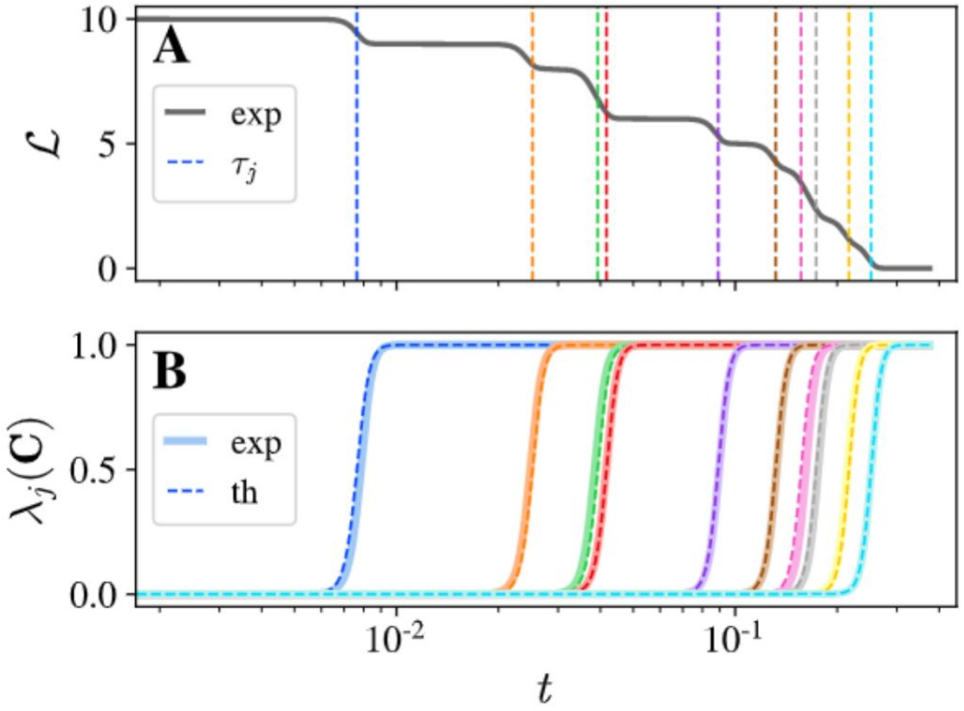
with $\boldsymbol{S}(t) = diag(s_1(t), ..., s_d(t))$ and



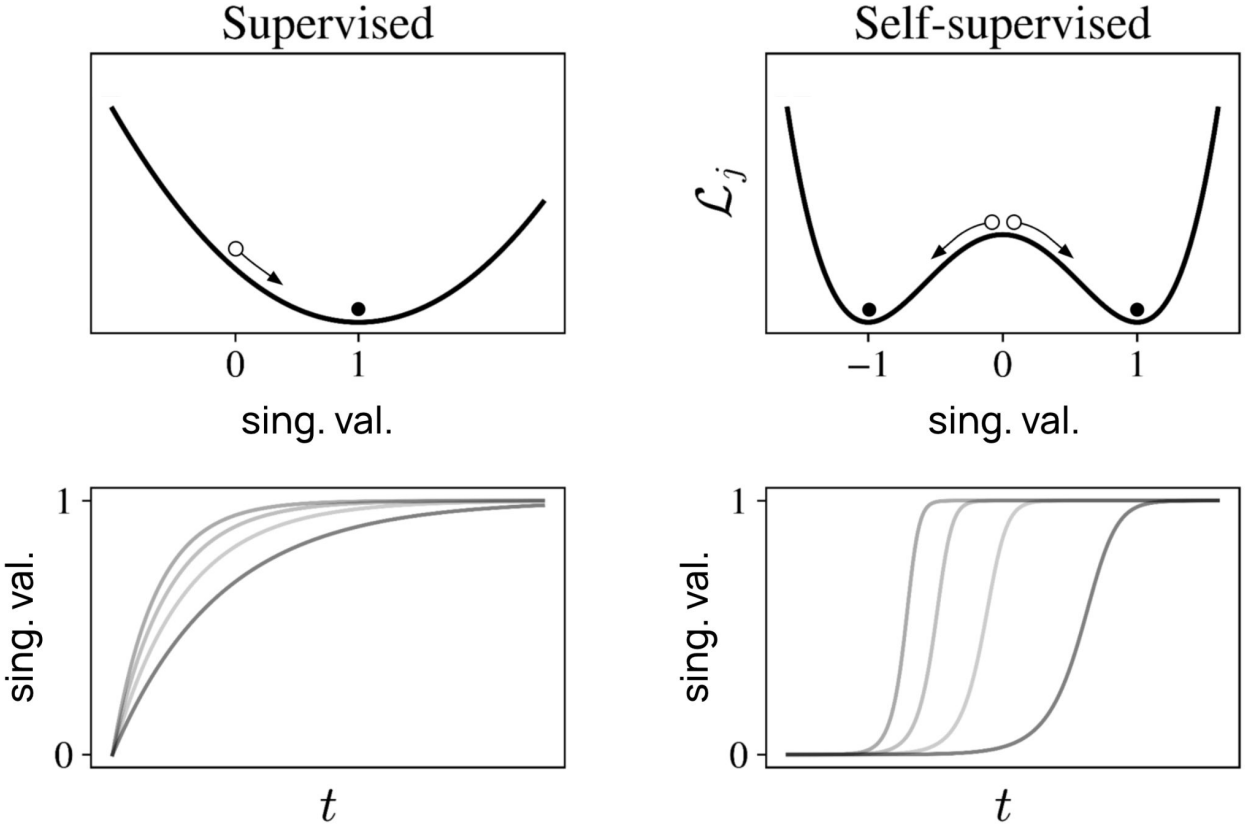
$$s_j(t) = \frac{e^{4\gamma_j t}}{\sqrt{s_j^{-2}(0) + (e^{8\gamma_j t} - 1)\gamma_j}}. \tag{10}$$

j-th eigenvalue of $\boldsymbol{\Gamma}$

From *generic small init*, these dynamics follow the aligned trajectory!



Representation learning is a process of *symmetry breaking.*



$$\dot{s_j} = \gamma_j(s_j^* - s_j)$$

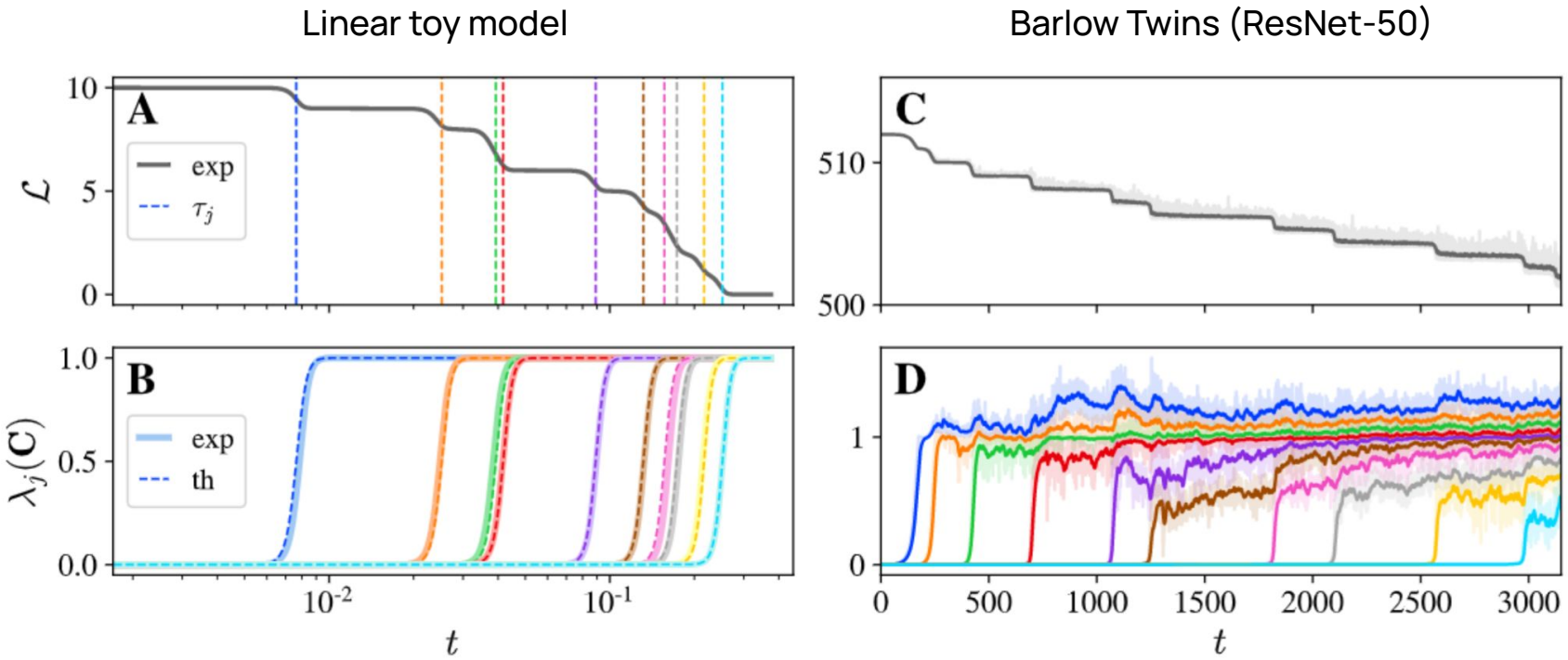
$$\dot{s_j} = \gamma_j s_j(1 - s_j^2)$$

It's kernel time

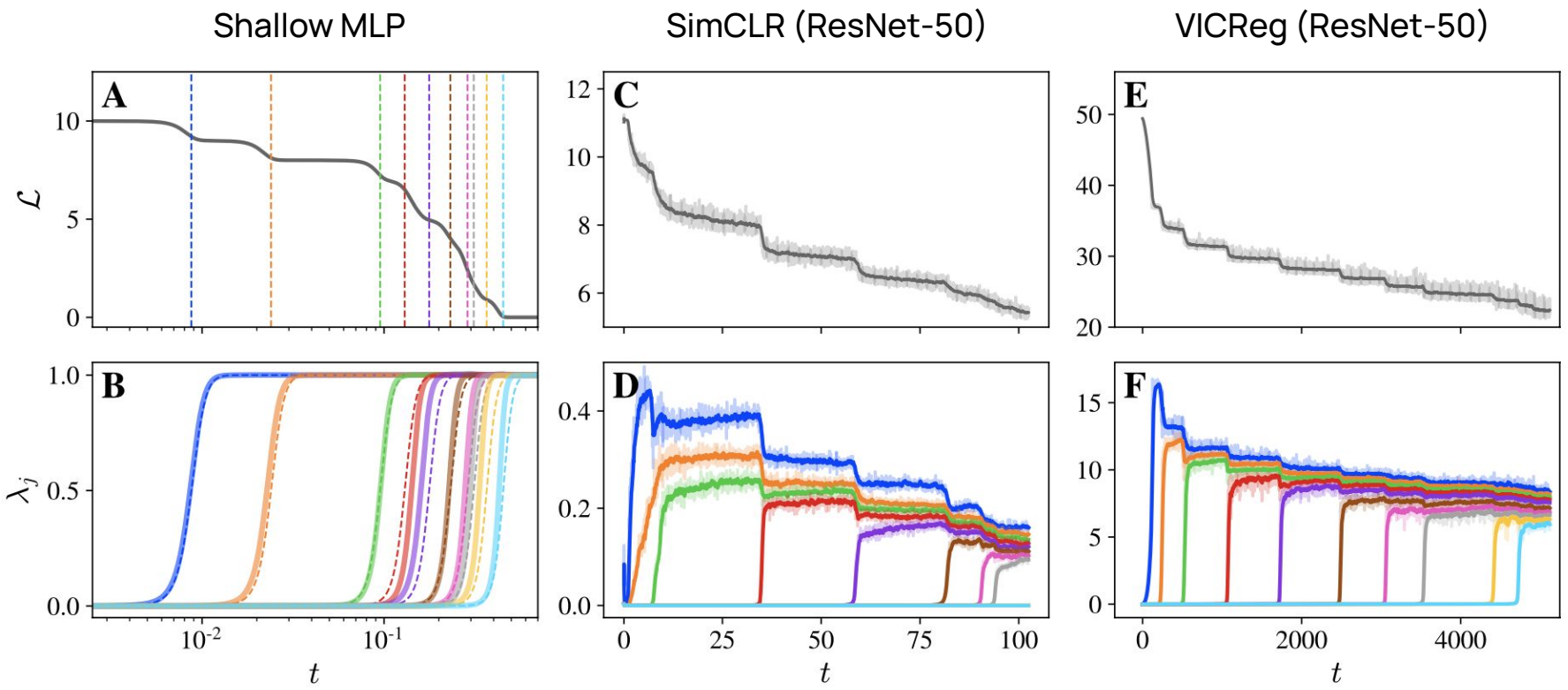
To kernelize, rephrase everything in terms of inner products $\boldsymbol{x}^T\boldsymbol{x}'$, then sub in $\mathrm{K}(\mathrm{x},\mathrm{x}') \equiv \boldsymbol{x}^T\boldsymbol{x}'$.

End of theory. Let’s check against ResNets.

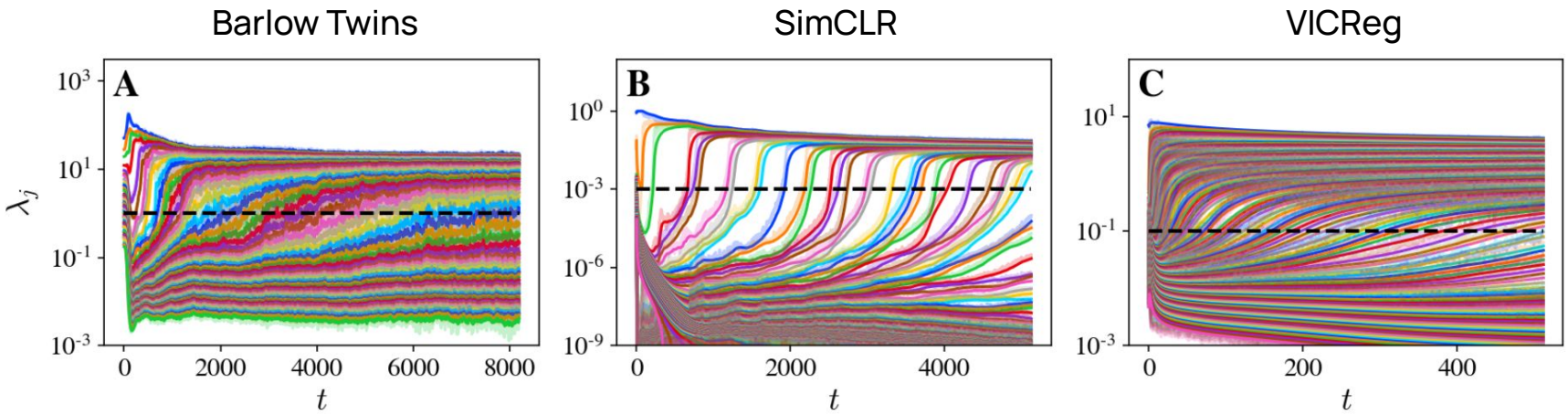
ResNets with small init show stepwise learning on STL-10.



ResNets with small init show stepwise learning on STL-10 (cont.).



…and you can still see the stepwise behavior with regular init!



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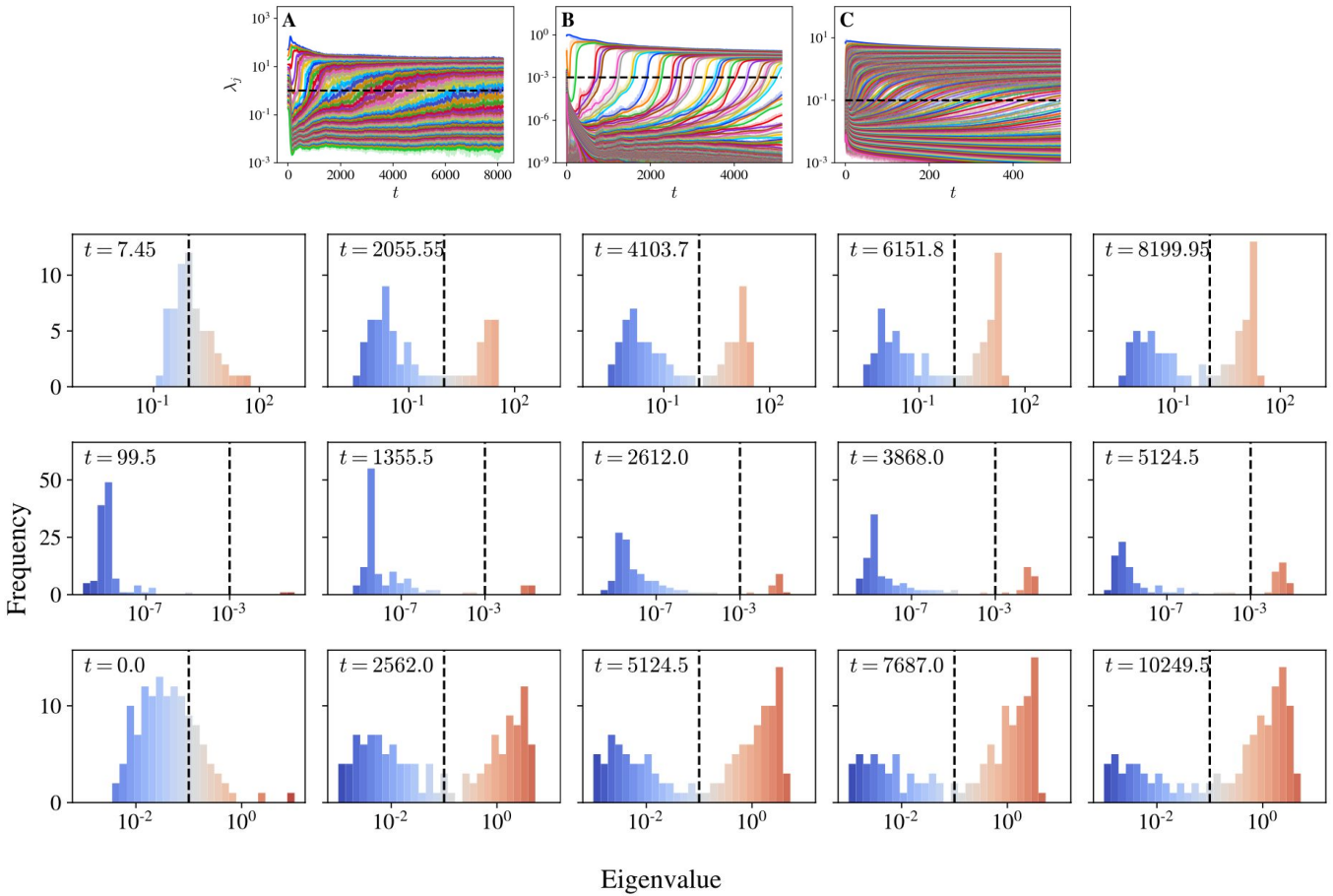


Future directions

Training SSL is famously slow. Can we speed it up?

Interpretability of top eigendirections?

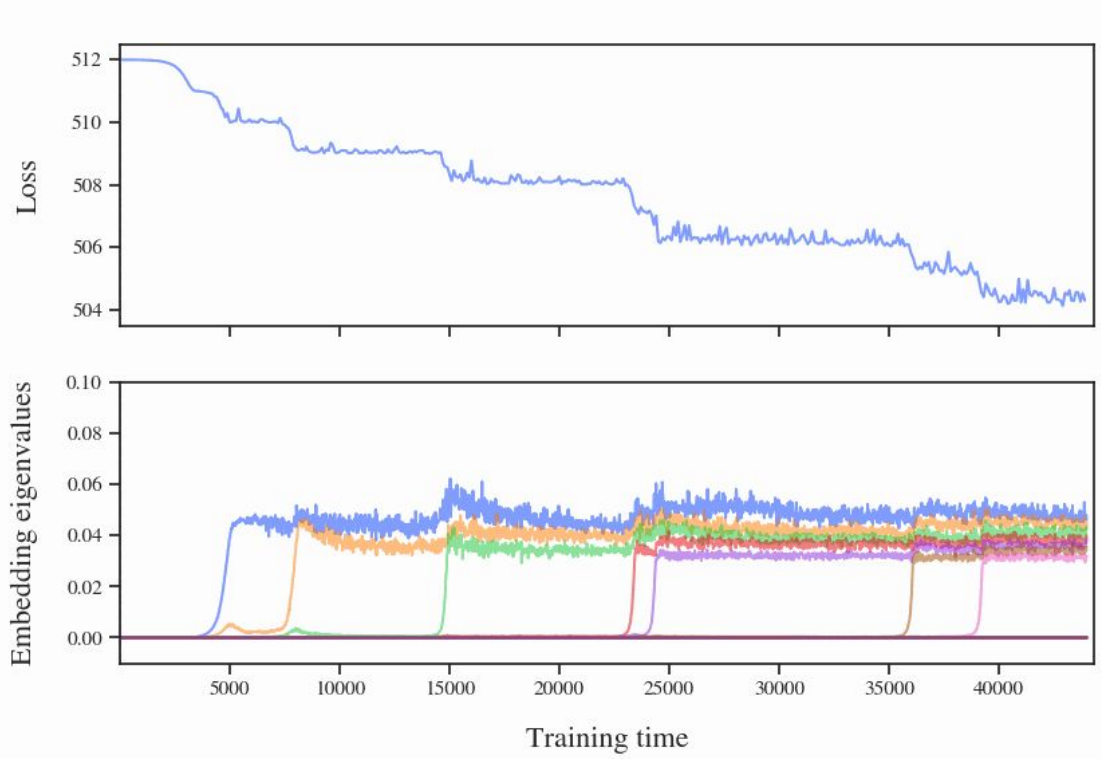
Stepwise learning in other settings? LLMs?

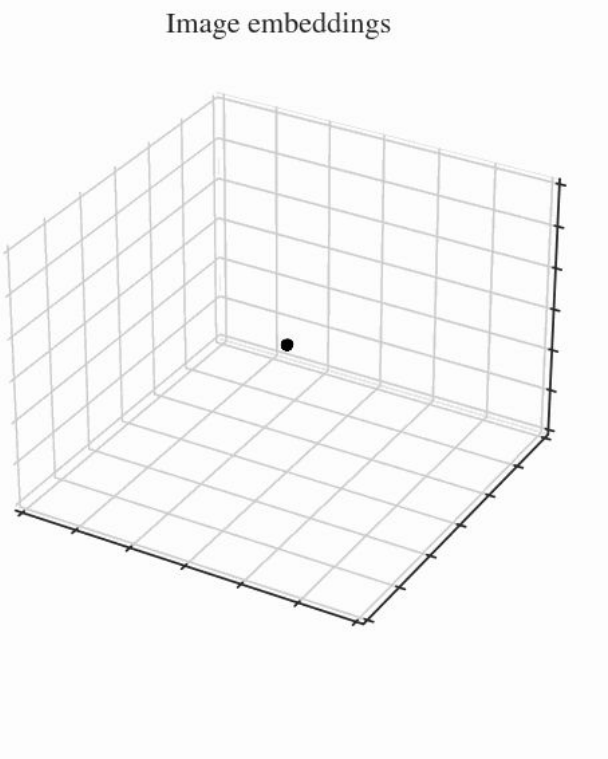
Broader lessons

1) Let's study (self/un)-supervised learning

2) It's worth collaborating with experimentalists

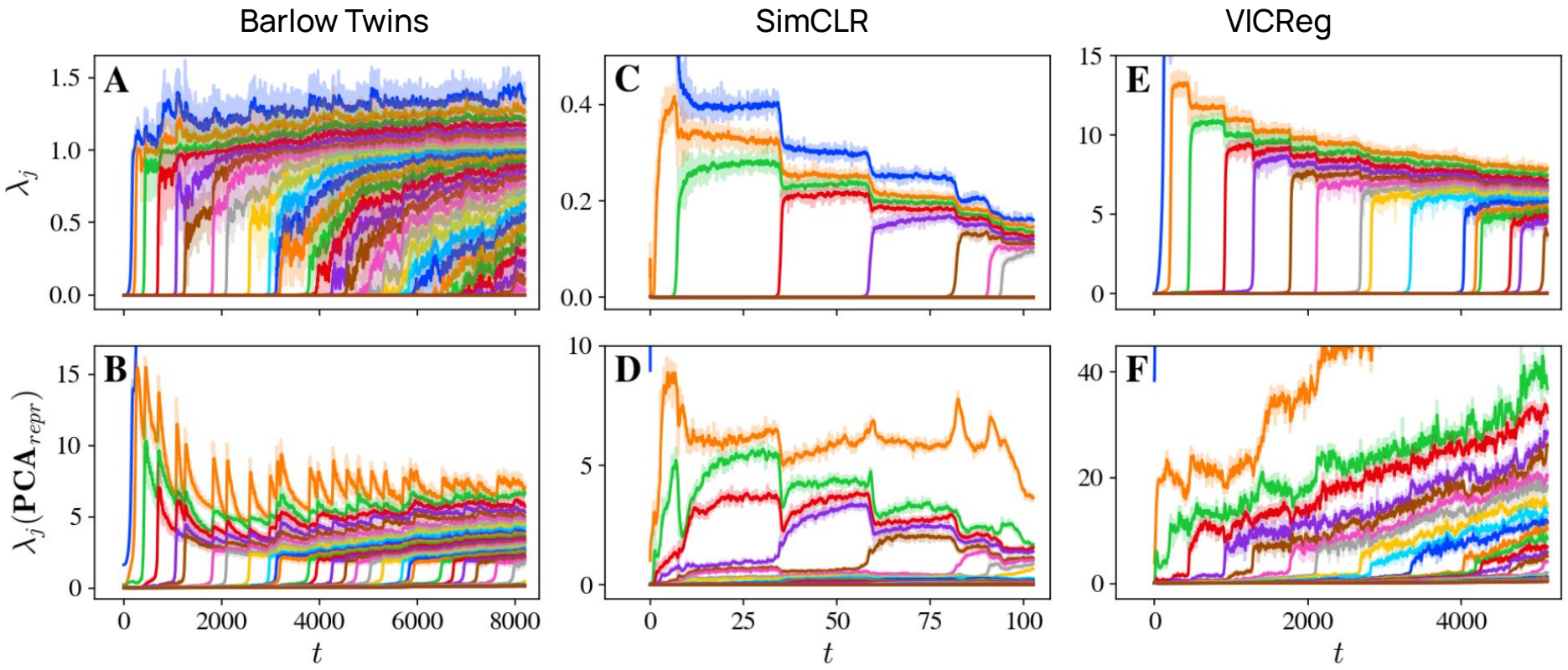
Summary: SOTA self-supervised systems show striking steps ('specially starting small)





(backups)

...and you can see it in *hidden representations* too!



We can mostly predict embeddings from the final NTK.

Procedure:

- Train a ResNet on full STL-10 dataset from small init.
- Measure eNTK after training on 1k positive pairs.
- Compute predicted embeddings from the eNTK.
- Compute inner product of true + predicted embedding subspaces.

	BT	SimCLR	VICReg	(random subspaces)
$\mathrm{a}(\boldsymbol{P}_{\mathrm{exp}}, \boldsymbol{P}_{\mathrm{th}})$	0.615	0.517	0.592	0.025

Not perfect, but pretty good agreement!