

Generalization and Optimization in Symmetry-Preserving ML: Sample Complexity and Implicit Bias

Wei Zhu

University of Massachusetts Amherst

Boston Symmetry Day
MIT

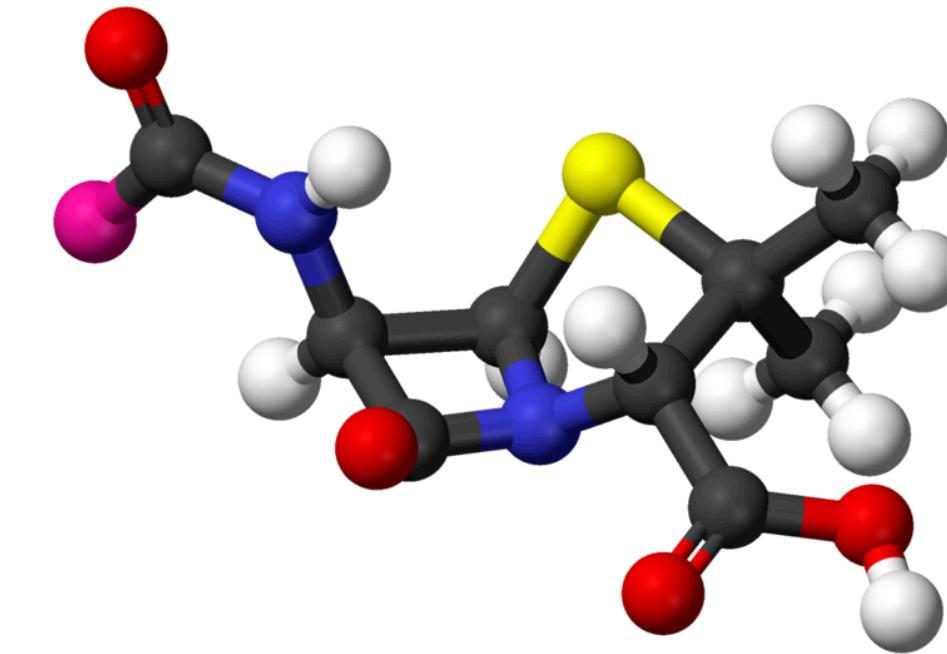
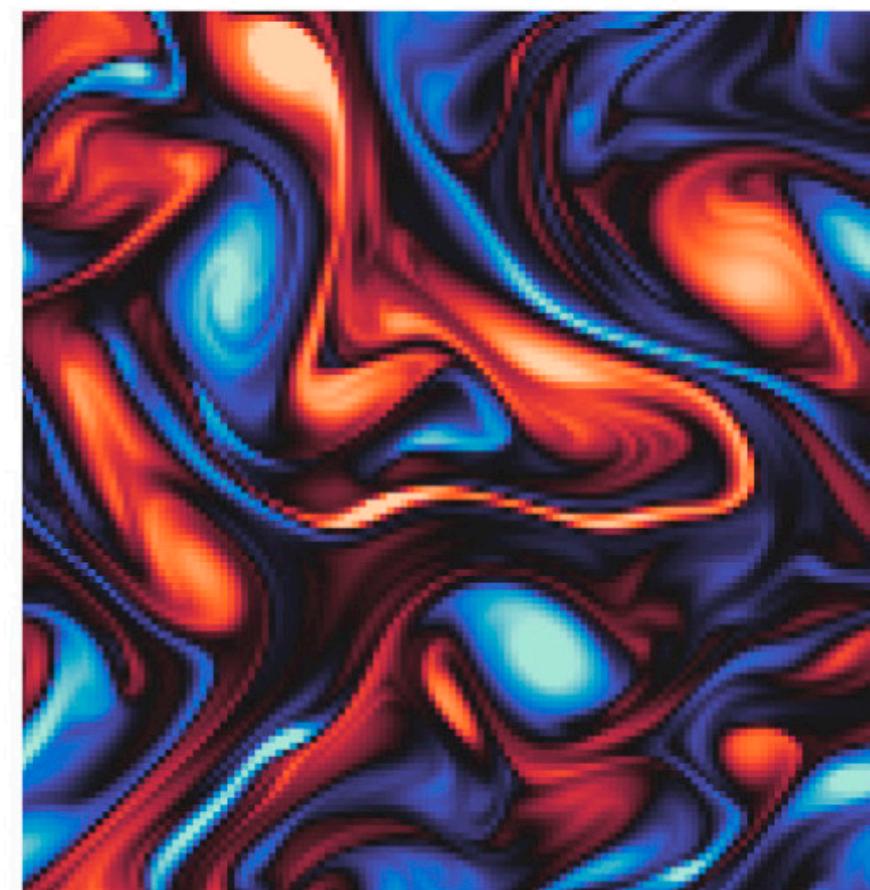
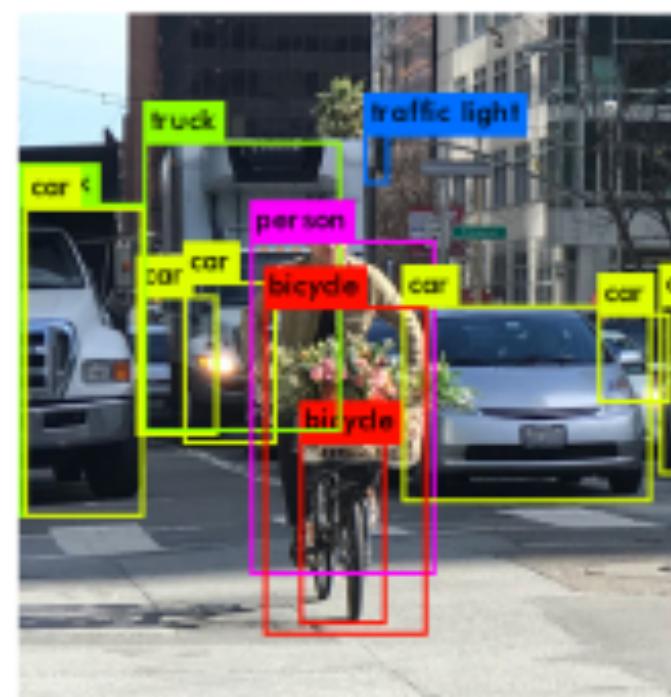
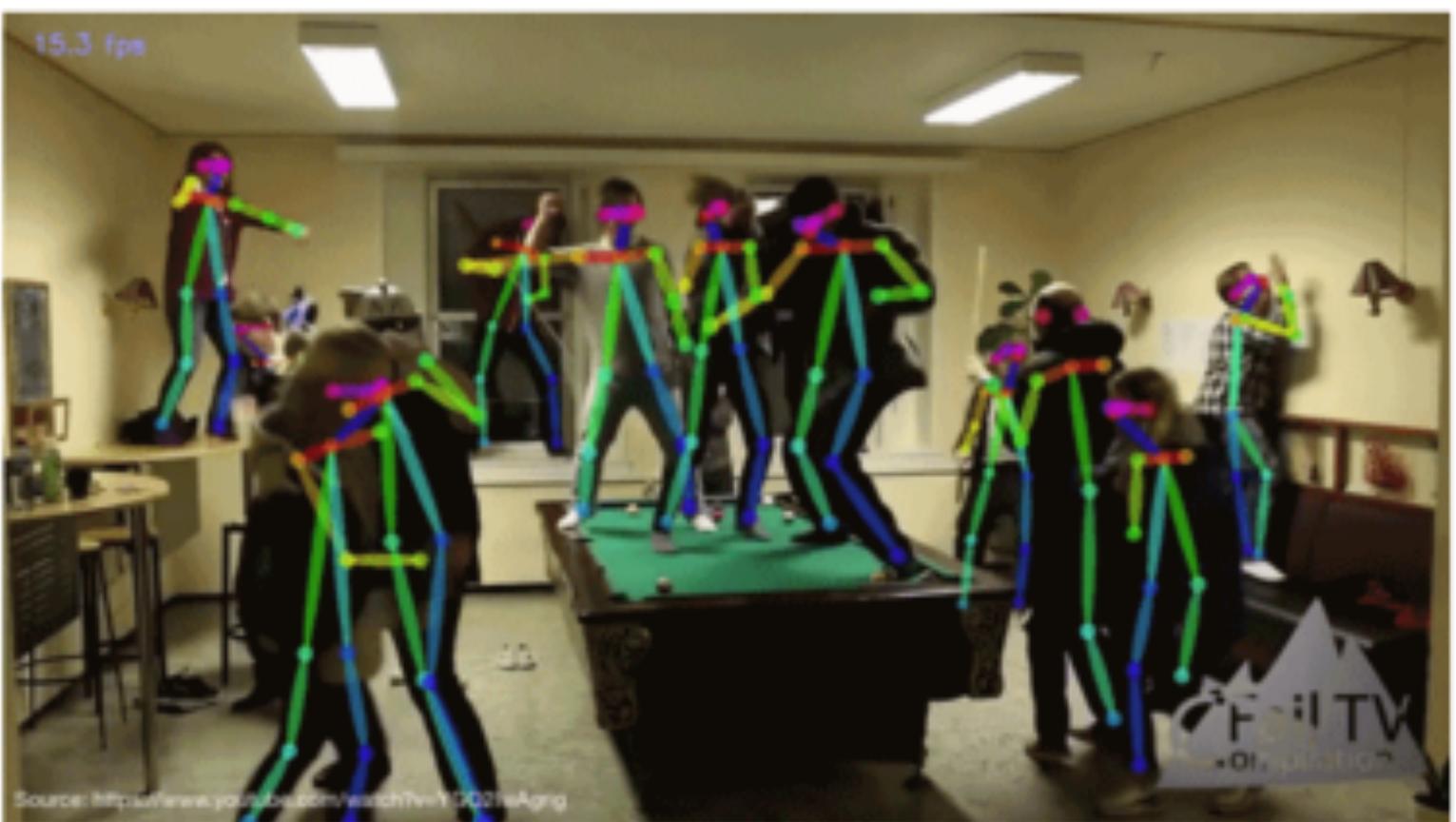
November 3, 2023



Joint work with many people, but mostly **Ziyu Chen** (UMass Amherst)



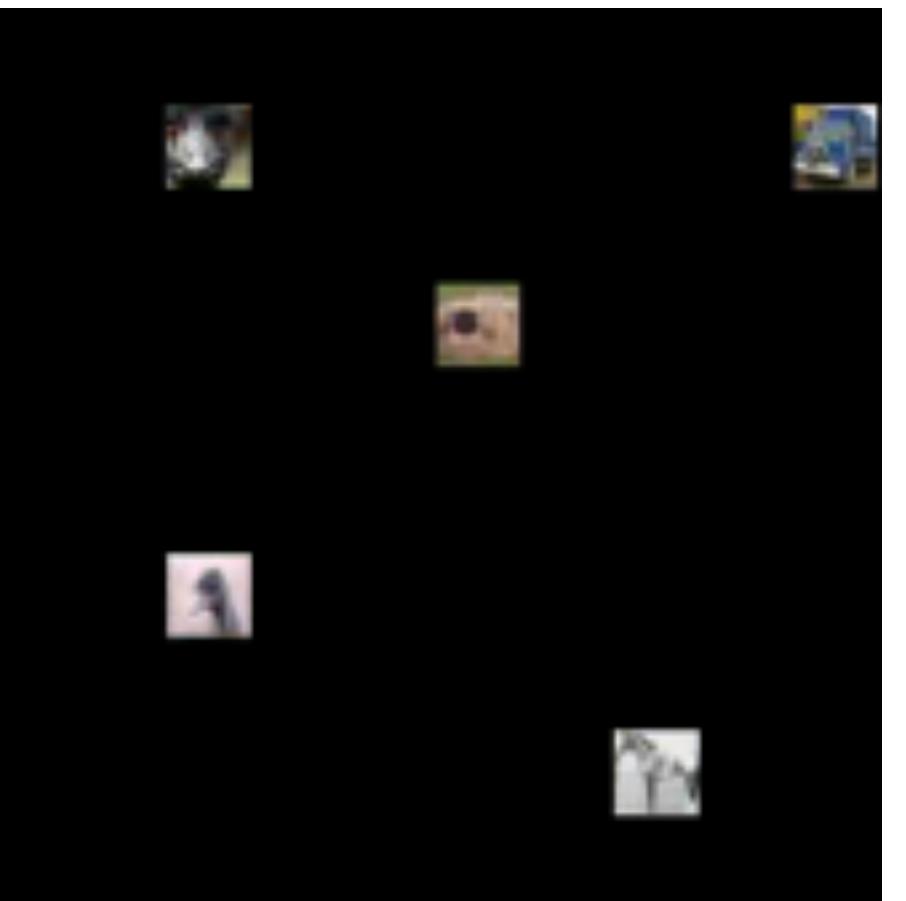
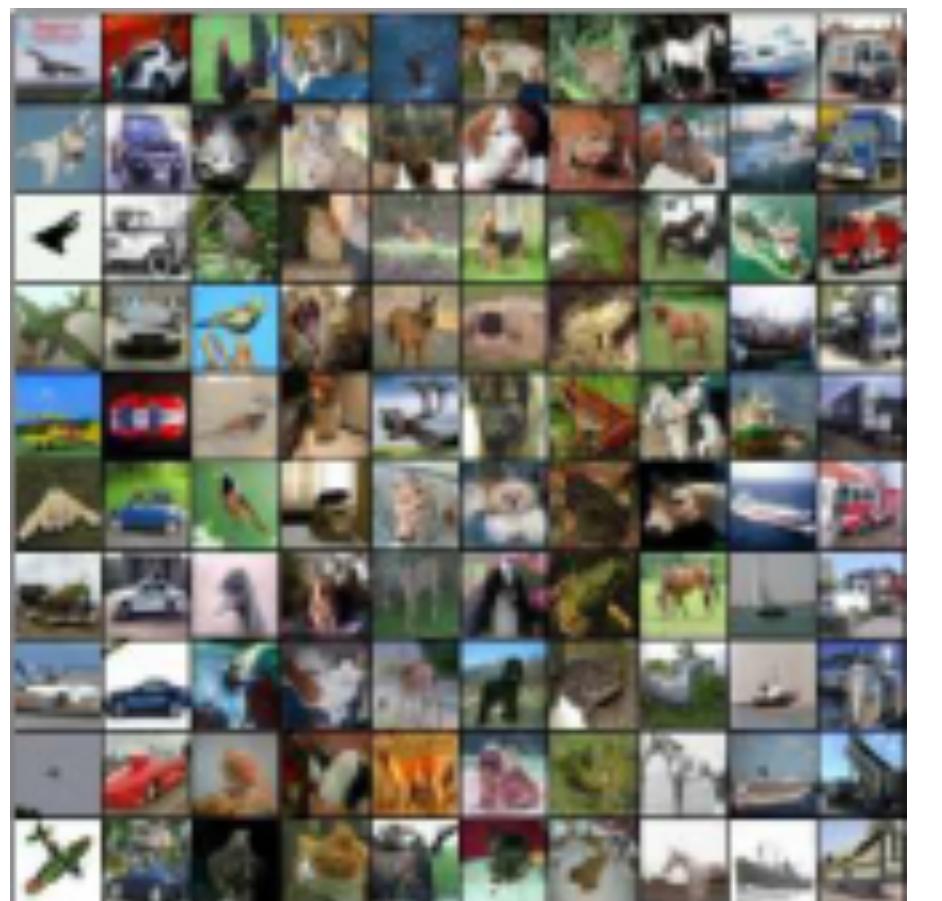
Symmetry is everywhere



Missing pieces

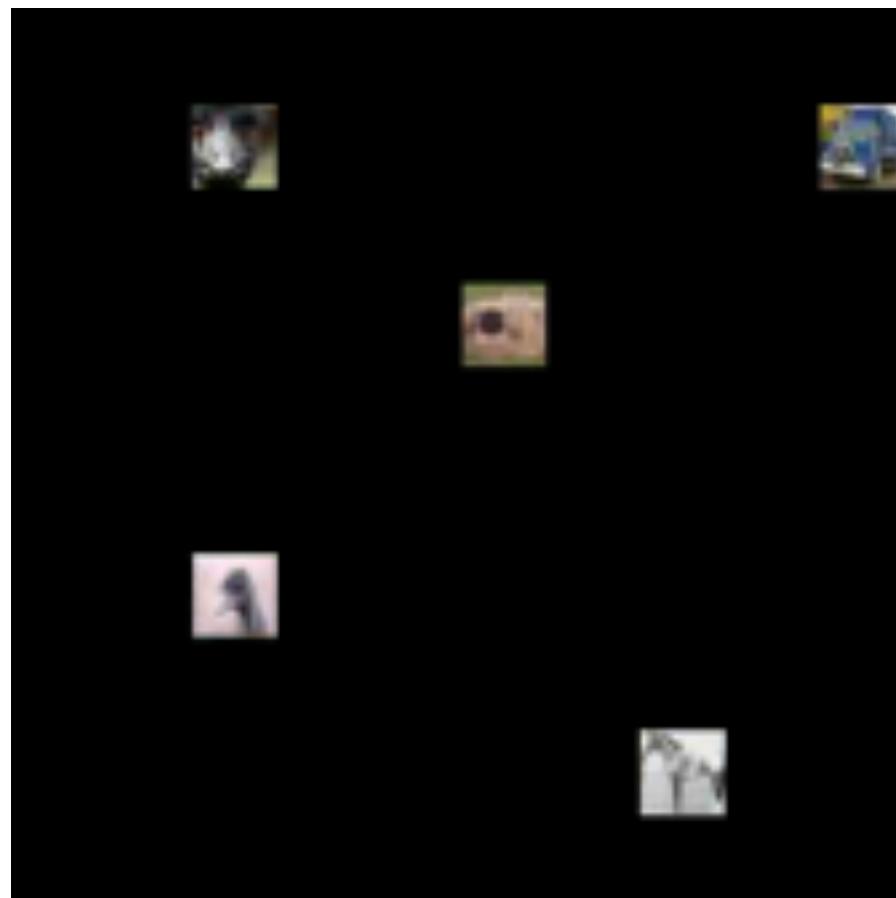
Missing pieces

- **Exact quantification of the improvement**
 - **Sample complexity** and **error bound.**



Missing pieces

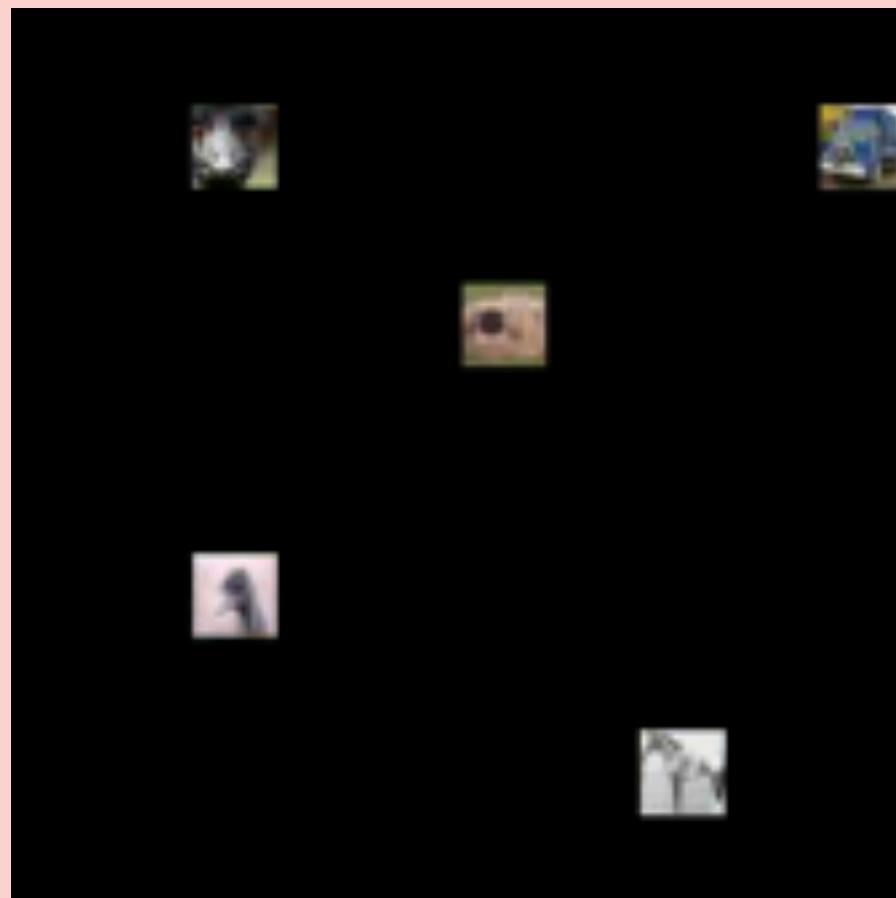
- Exact quantification of the improvement
 - Sample complexity and error bound.
- Does it converge? To what solution?
 - Training dynamics of equivariant models



$$\mathbf{W}^* = \arg \min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

Missing pieces

- Exact quantification of the improvement
 - Sample complexity and error bound.
- Does it converge? To what solution?
 - Training dynamics of equivariant models



$$\mathbf{W}^* = \arg \min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

Symmetry-preserving GANs and their improved sample complexity

- J. Birrell, M.A. Katsoulakis, L. Rey-Bellet, **W. Zhu**. “Structure-preserving GANs”. *ICML* (2022)
- Z. Chen, M.A. Katsoulakis, L. Rey-Bellet, **W. Zhu**. “Sample complexity of probability divergences under group symmetry”. *ICML* (2023)

Generative adversarial networks (GANs)

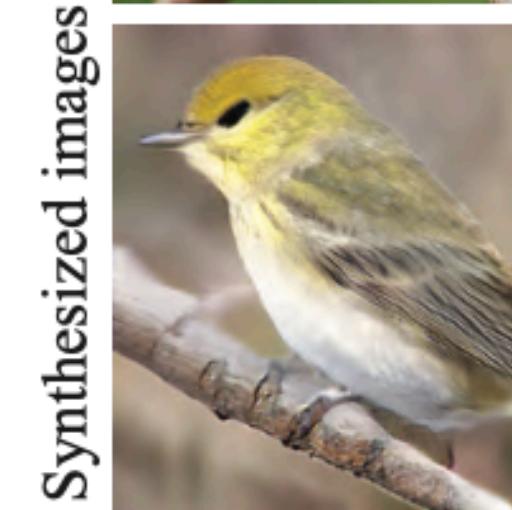


StyleGAN2, Karras et al., CVPR 2020



StyleGAN3, Karras et al., NeurIPS 2021

This small bird has a yellow crown and a white belly.



This bird has a blue crown with white throat and brown secondaries.



People at the park flying kites and walking.



The bathroom with the white tile has been cleaned.



DM-GAN, Zhu et al., CVPR 2019

Generative adversarial networks (GANs)

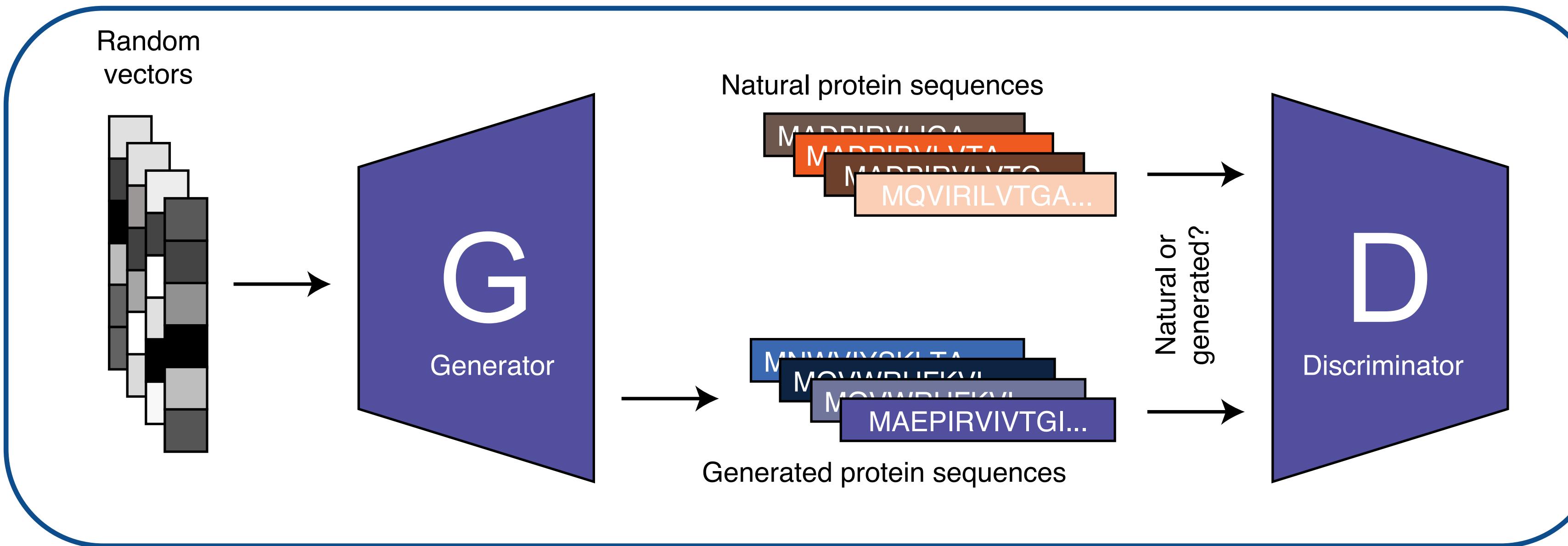


Figure: Repecka et al., *Nature Machine Intelligence* 2021

Generative adversarial networks (GANs)

- GANs use a pair of networks to learn (to sample from) an unknown probability distribution.

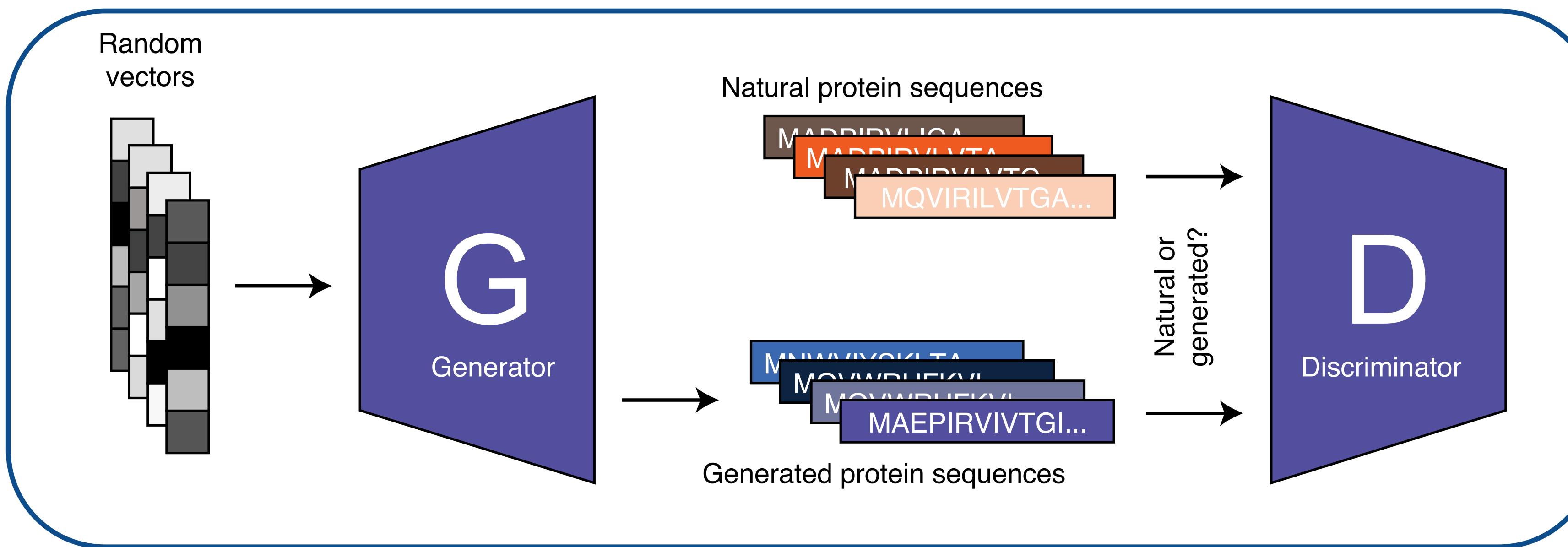


Figure: Repecka et al., *Nature Machine Intelligence* 2021

Generative adversarial networks (GANs)

- GANs use a pair of networks to learn (to sample from) an unknown probability distribution.
- **Zero-sum game** between **discriminator** and **generator**—“the players”.

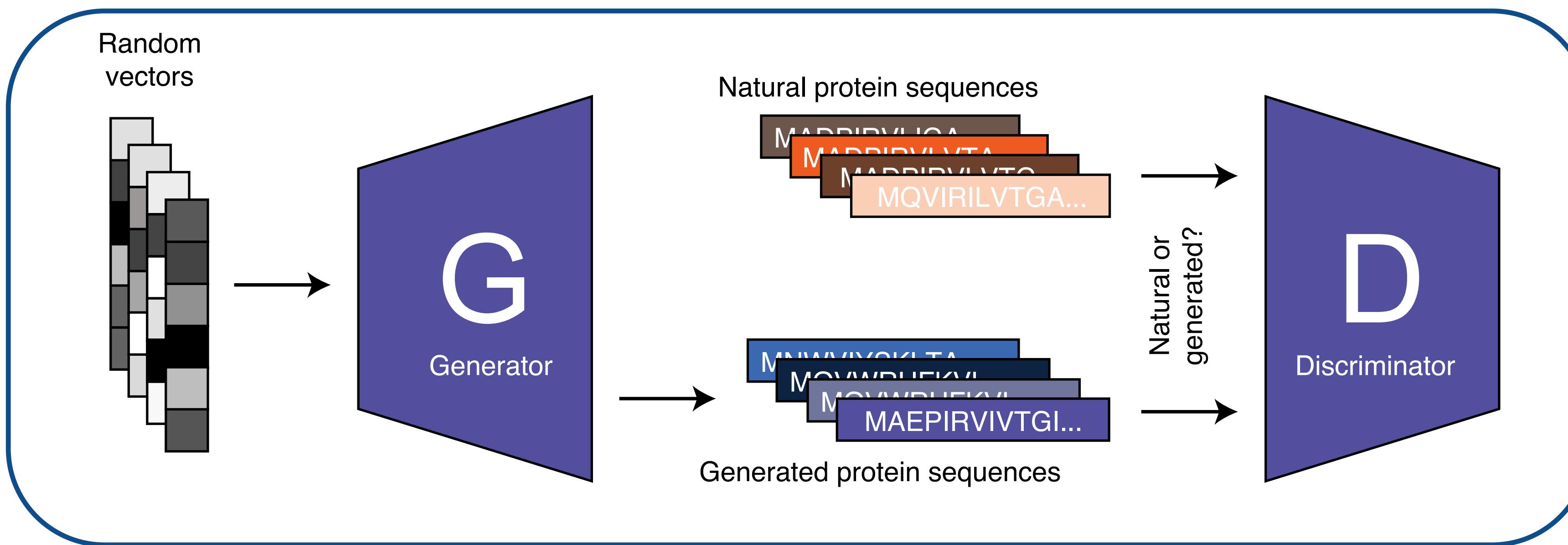


Figure: Repecka et al., *Nature Machine Intelligence* 2021

Generative adversarial networks (GANs)

- GANs use a pair of networks to learn (to sample from) an unknown probability distribution.
- **Zero-sum game** between **discriminator** and **generator**—“**the players**”.
- Game ends when the players reach consensus: “fake data” looks like the “real” data.

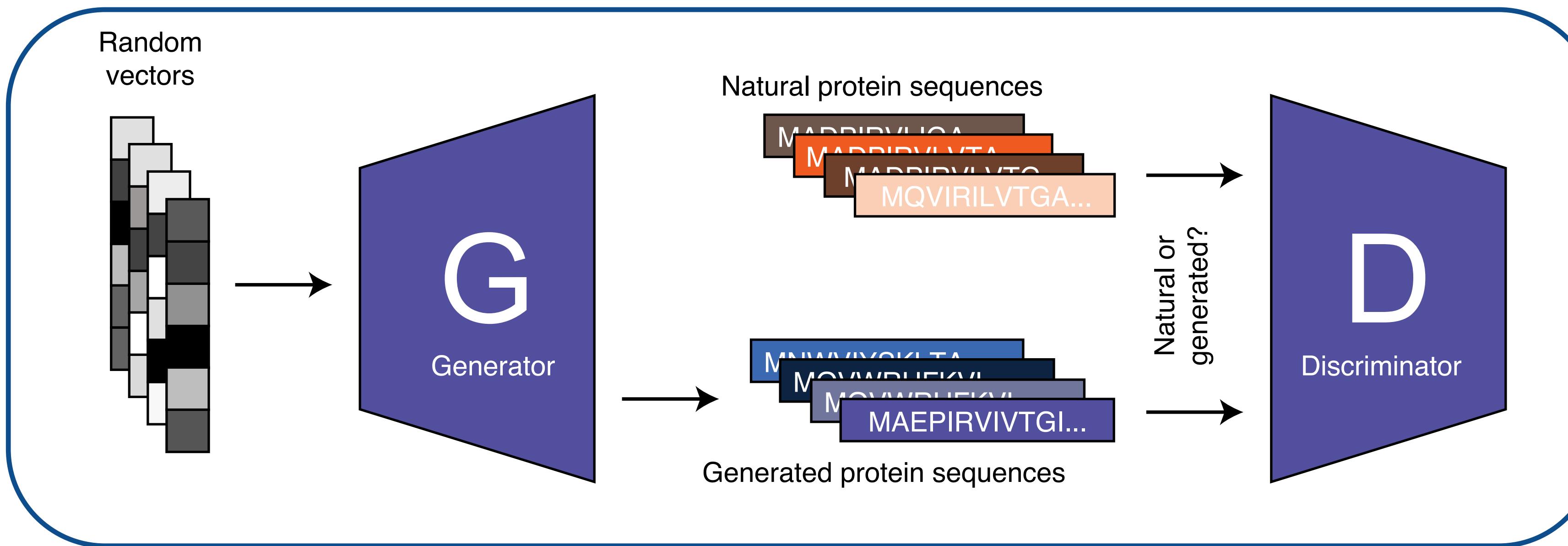
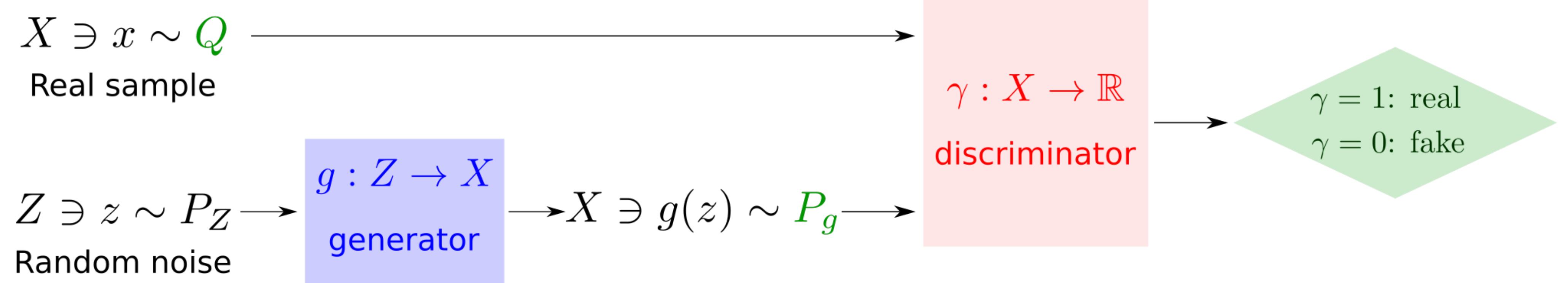
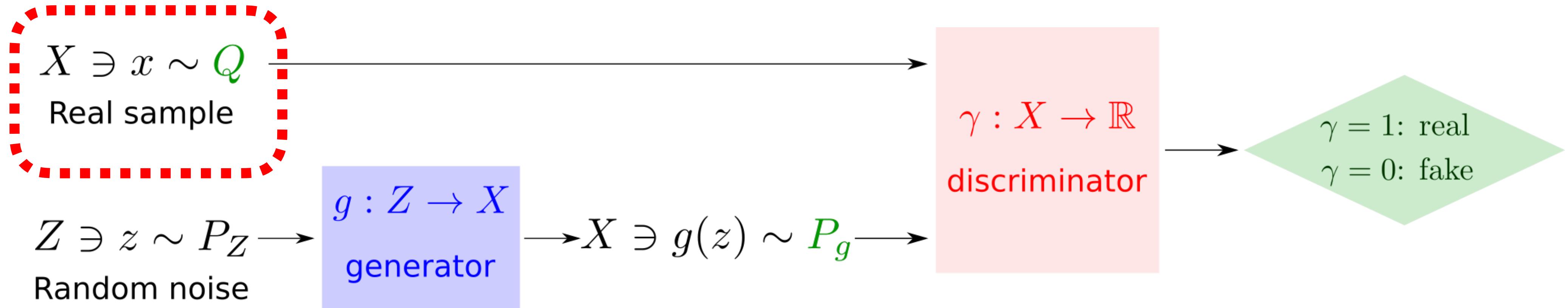


Figure: Repecka et al., *Nature Machine Intelligence* 2021

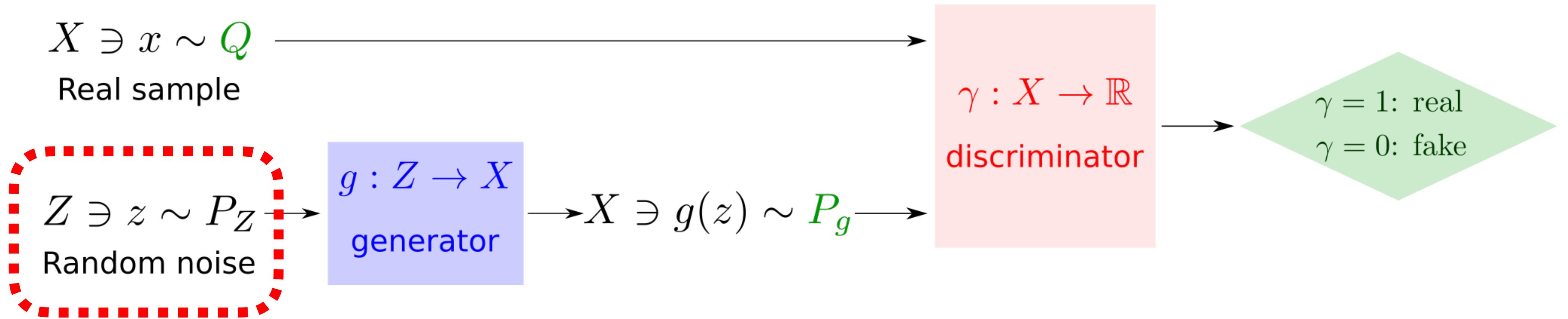
Generative adversarial networks (GANs)



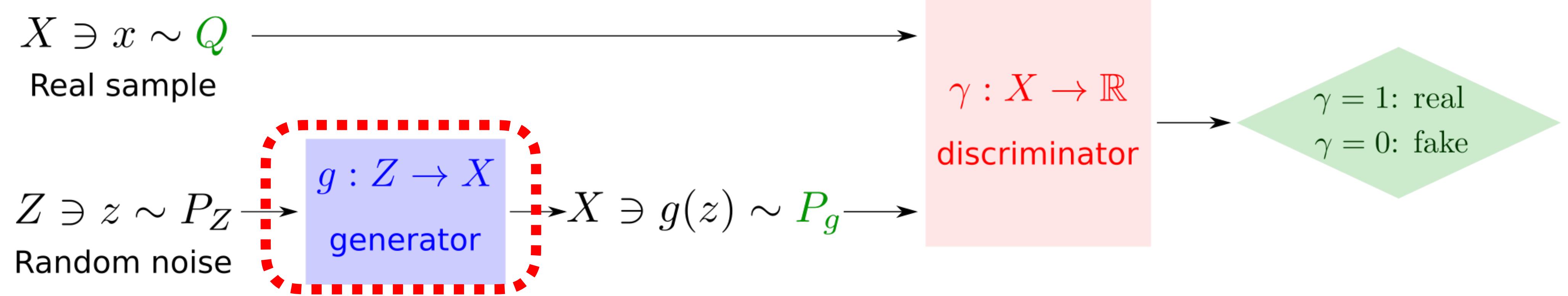
Generative adversarial networks (GANs)



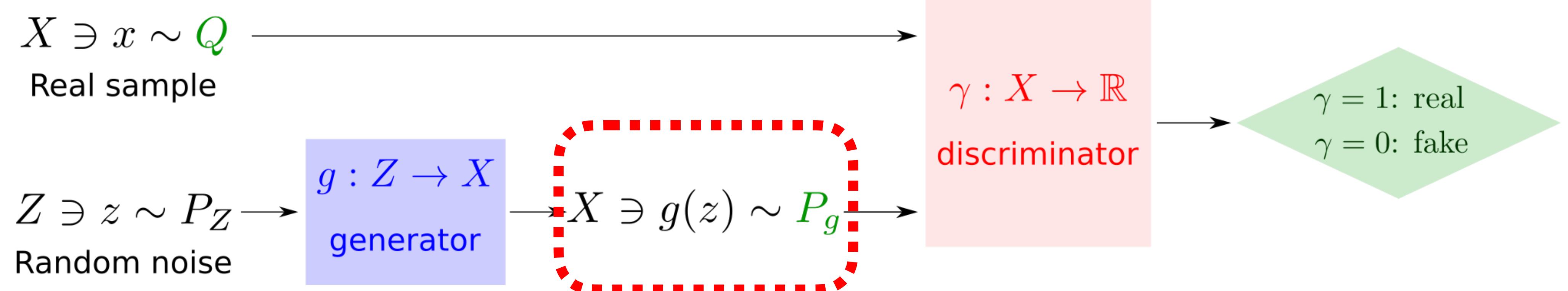
Generative adversarial networks (GANs)



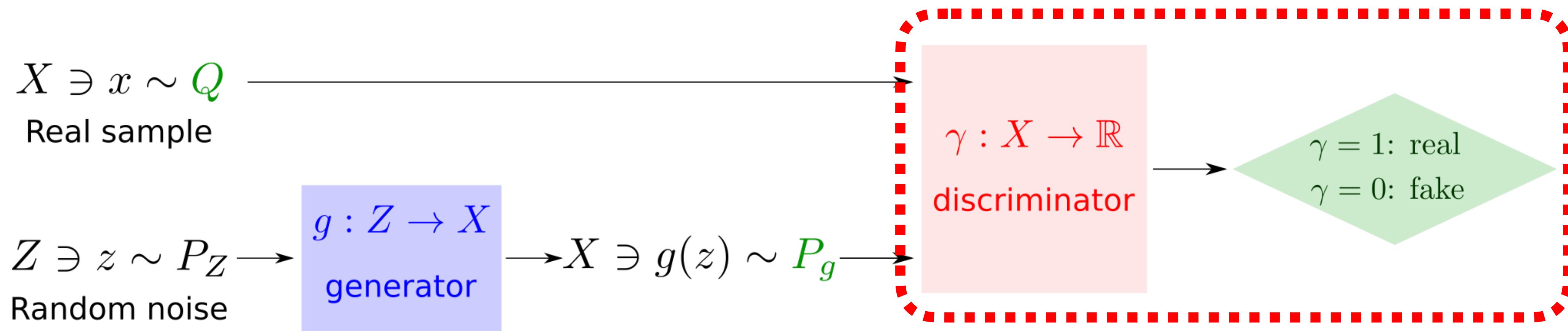
Generative adversarial networks (GANs)



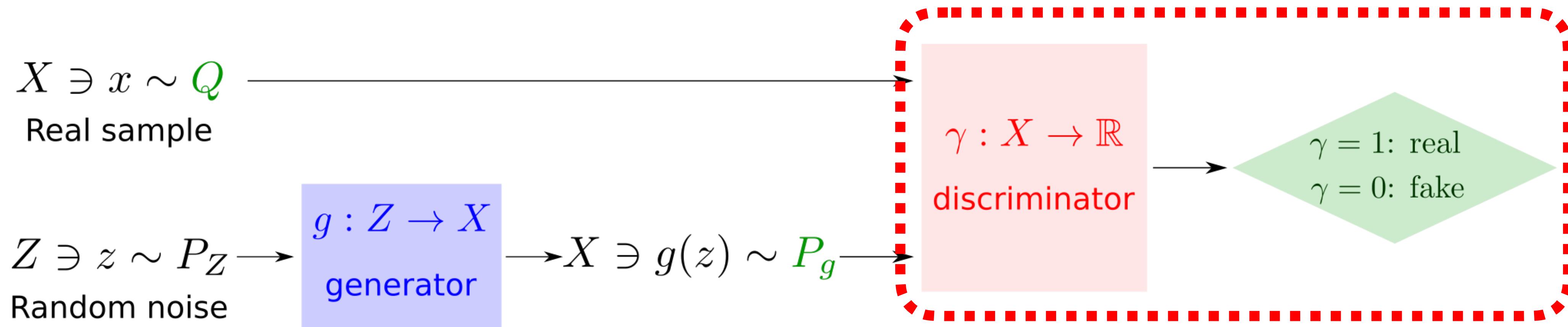
Generative adversarial networks (GANs)



Generative adversarial networks (GANs)



Generative adversarial networks (GANs)



- Mathematically, GAN is minimizing some divergence, $D_H^{\Gamma}(Q||P_g)$, between Q and P_g .
- $D_H^{\Gamma}(Q||P_g) = \max_{\gamma \in \Gamma} H(\gamma; Q, P_g)$ is determined by H and discriminators $\gamma \in \Gamma$.

$$\min_{g \in G} D_H^{\Gamma}(Q||P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g).$$

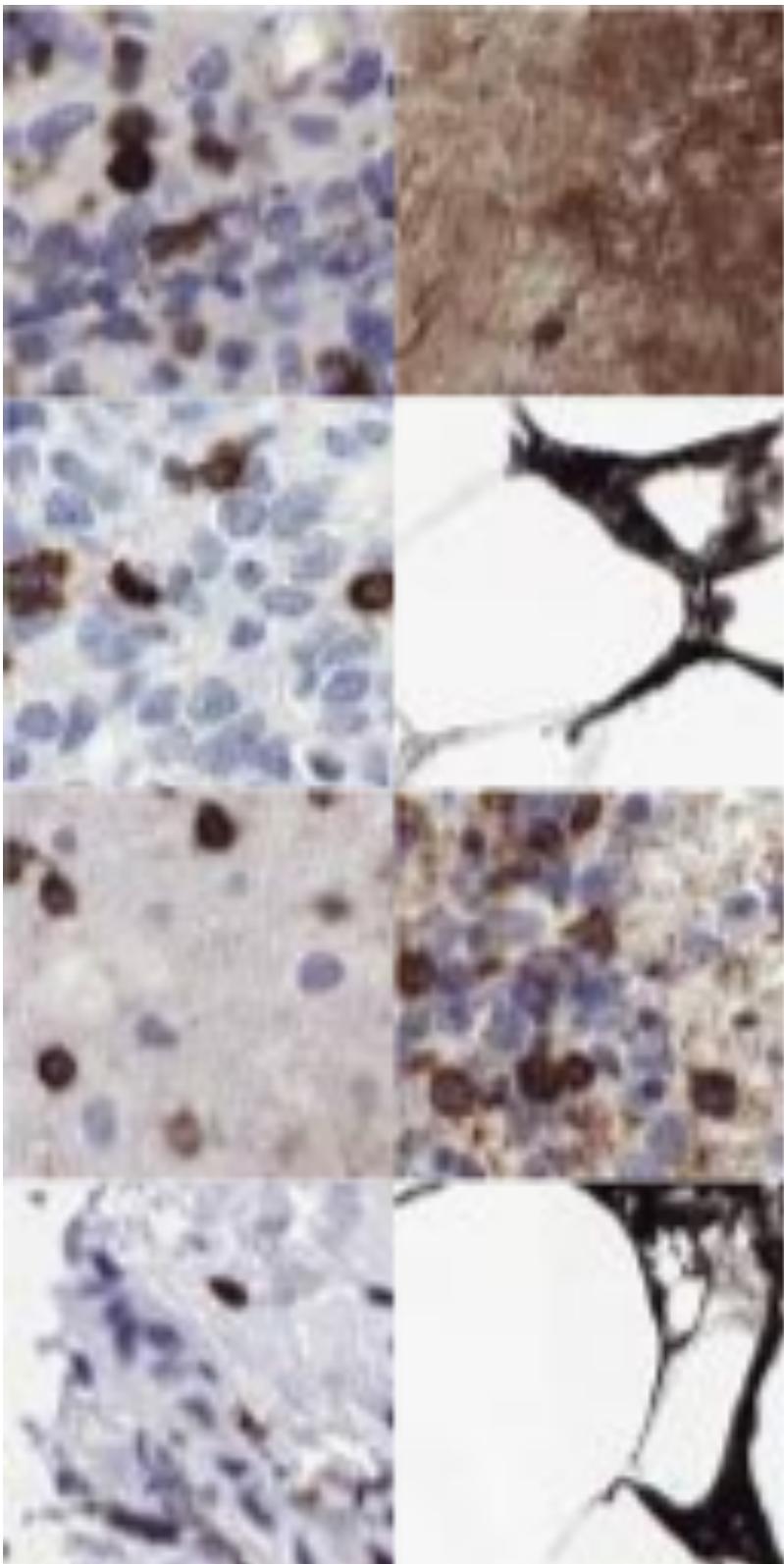
GAN is “probability divergence” minimization

$$\min_{g \in G} D_H^{\Gamma}(Q || P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g).$$

- The original GAN [Goodfellow et al., 2014]: Jensen–Shannon divergence (JSD).
- f -divergences: $D_f(Q || P) = \sup_{\gamma \in \mathcal{M}_b(X)} \{\mathbb{E}_Q[\gamma] - \mathbb{E}_P[f^*(\gamma)]\}$. (KL, JSD, etc.)
- Γ -IPM: $W^{\Gamma}(Q || P) = \sup_{\gamma \in \Gamma} \{\mathbb{E}_Q[\gamma] - \mathbb{E}_P[\gamma]\}$. (TV, Dudley metric, Wasserstein-1, MMD)
- Wasserstein metric and Sinkhorn divergence.

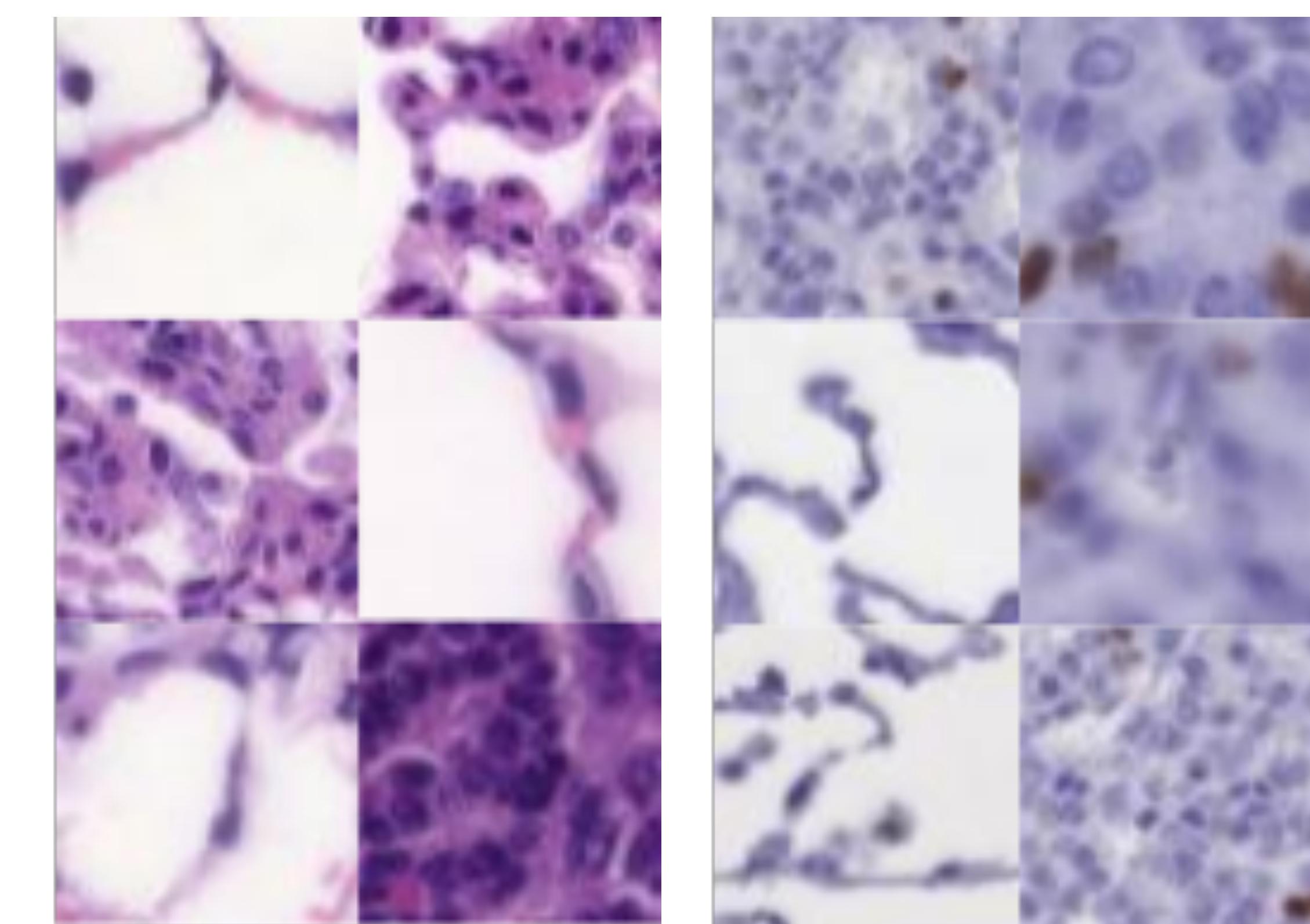
Structured target data & distribution Q

Q



LYSTO¹

1. *Ciompi et al., Zenodo 2019*
2. *Borovec et al., IEEE Transactions on Medical Imaging 2020*

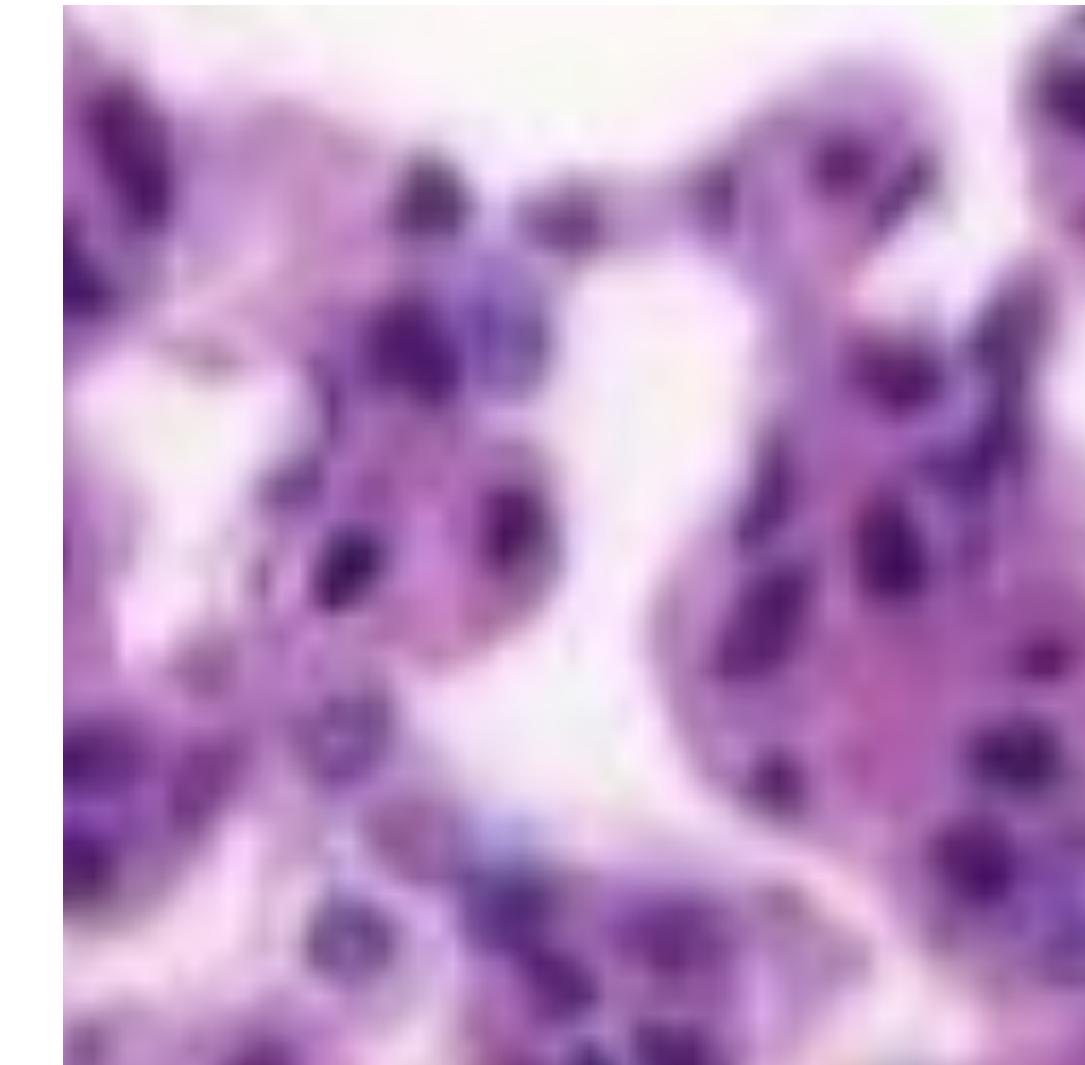


ANHIR²

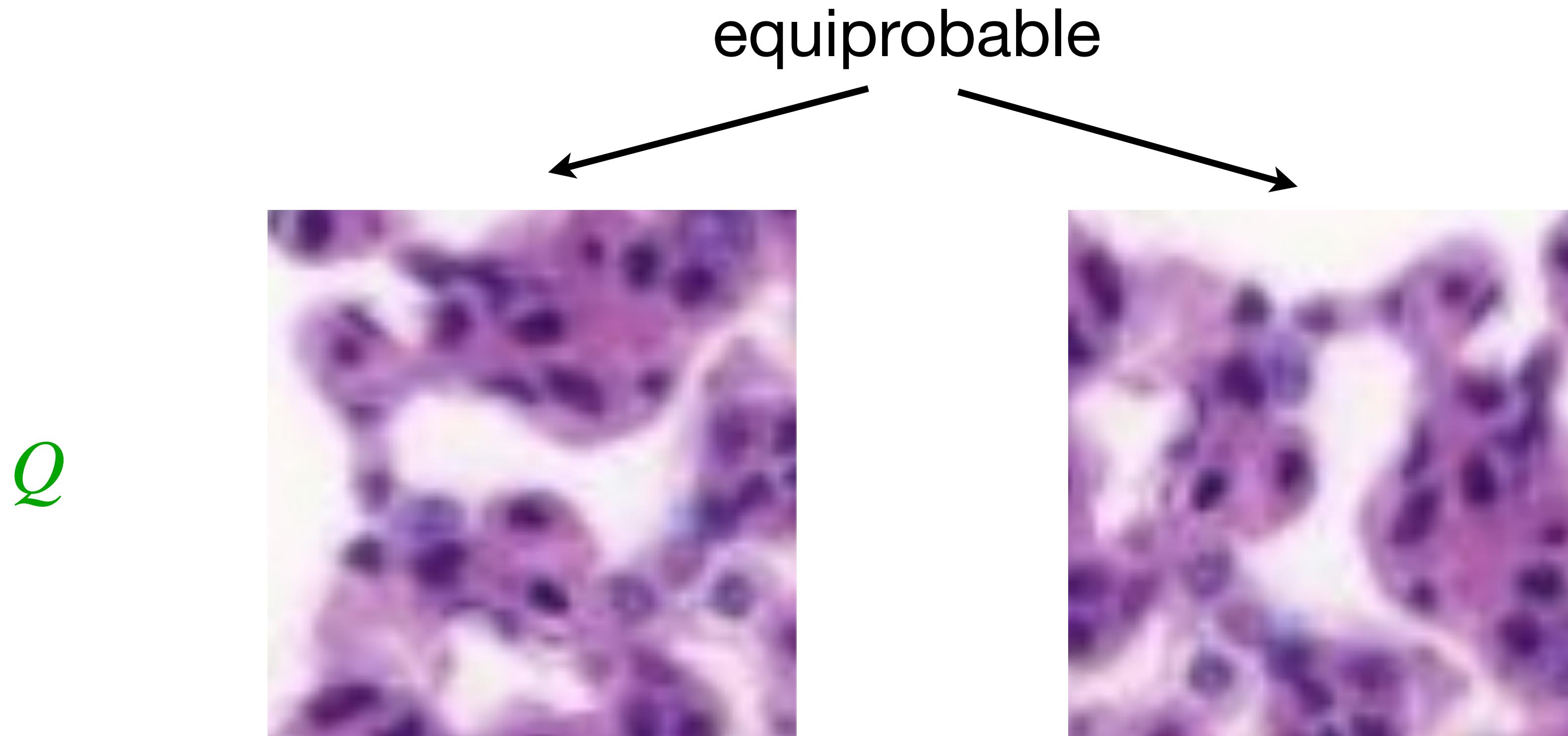
Structured target data & distribution \mathcal{Q}

\mathcal{Q}

equiprobable

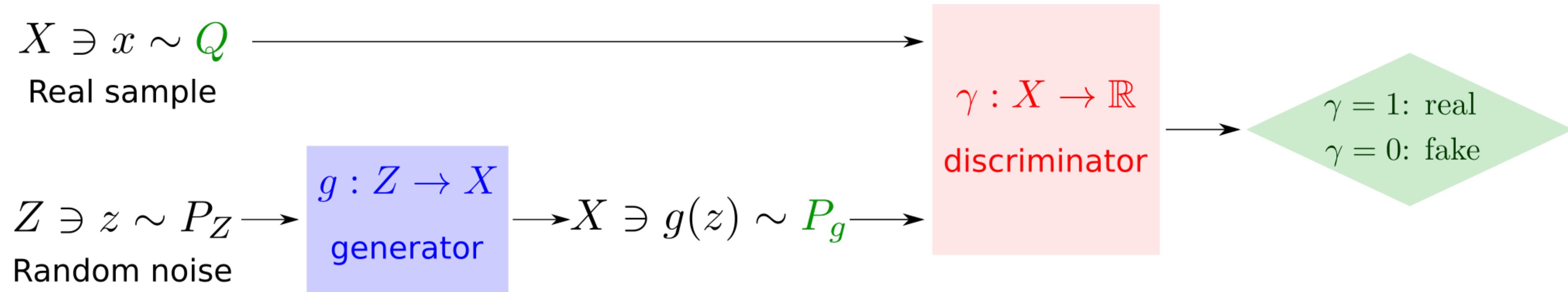


Structured target data & distribution Q

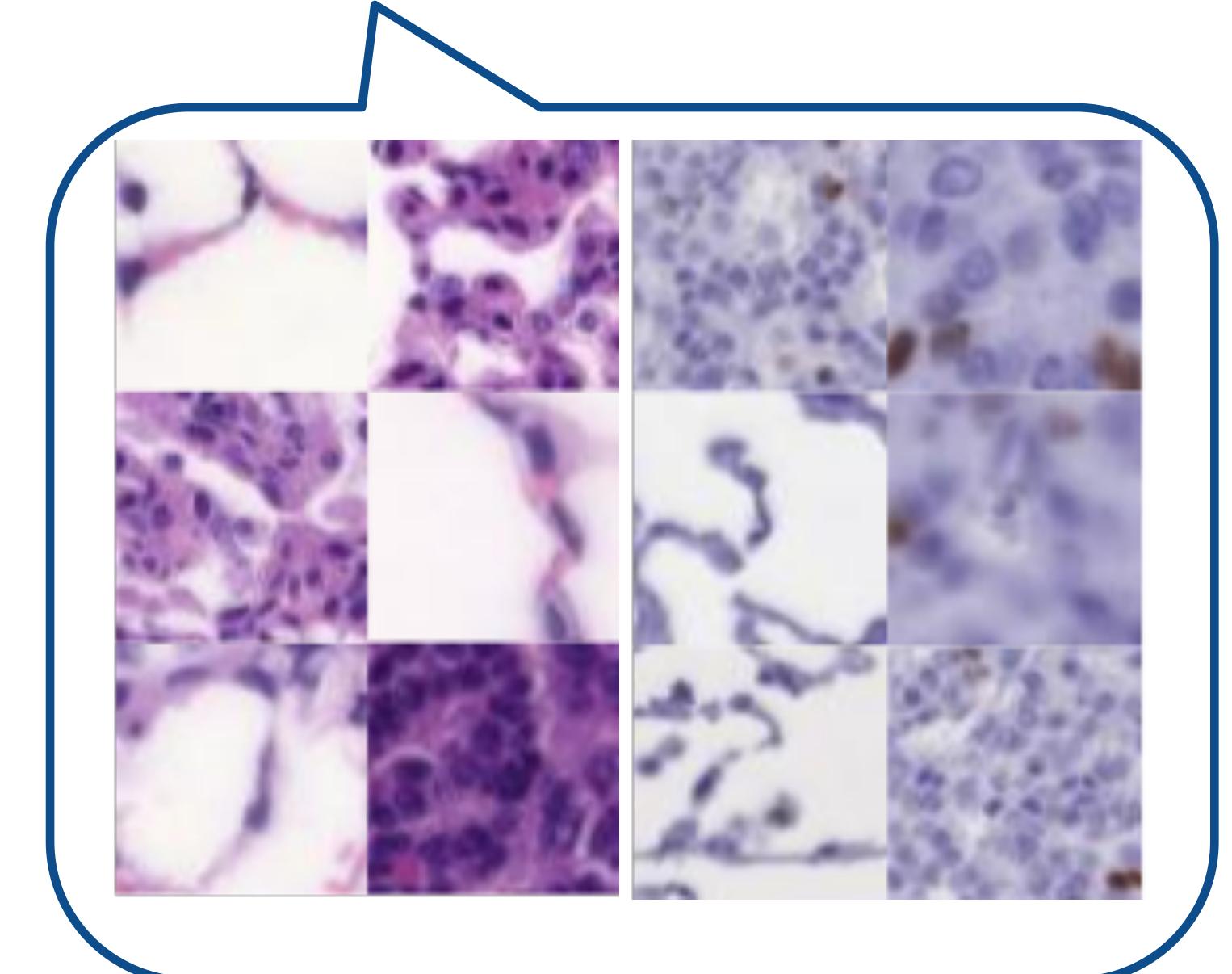


Question: how to build **embedded structure** into GAN players (generators and discriminators) for **data-efficient** distribution learning?

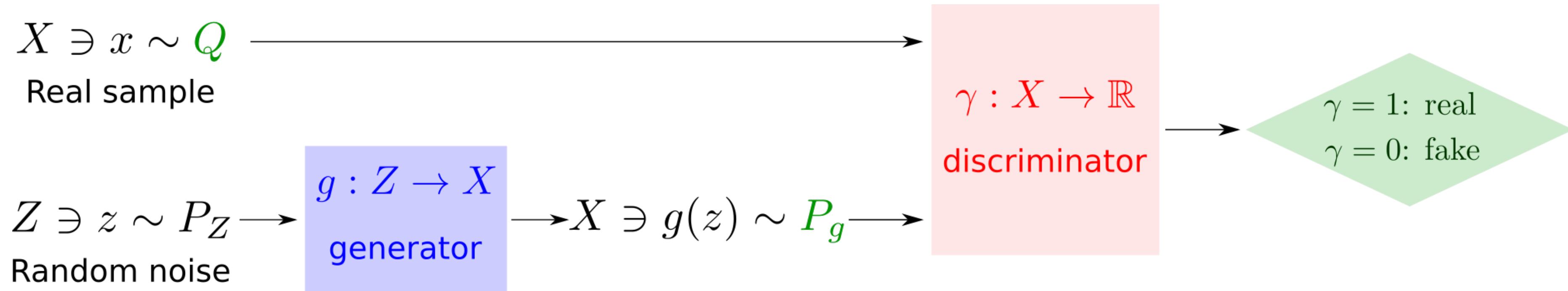
GAN with embedded structure



$$\min_{g \in G} D^\Gamma(Q \| P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g), \quad \underline{Q \text{ is } \Sigma\text{-invariant}}$$

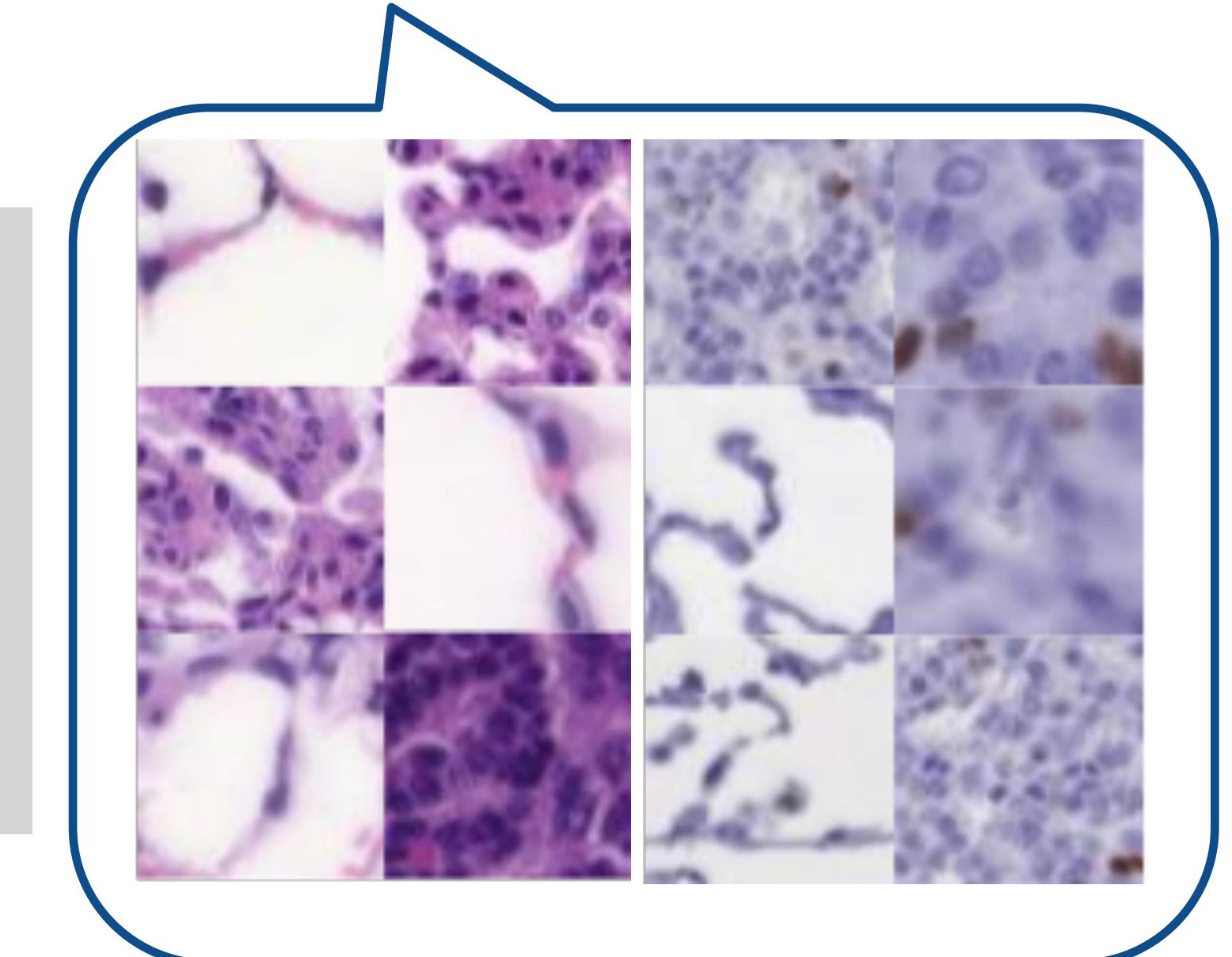


GAN with embedded structure

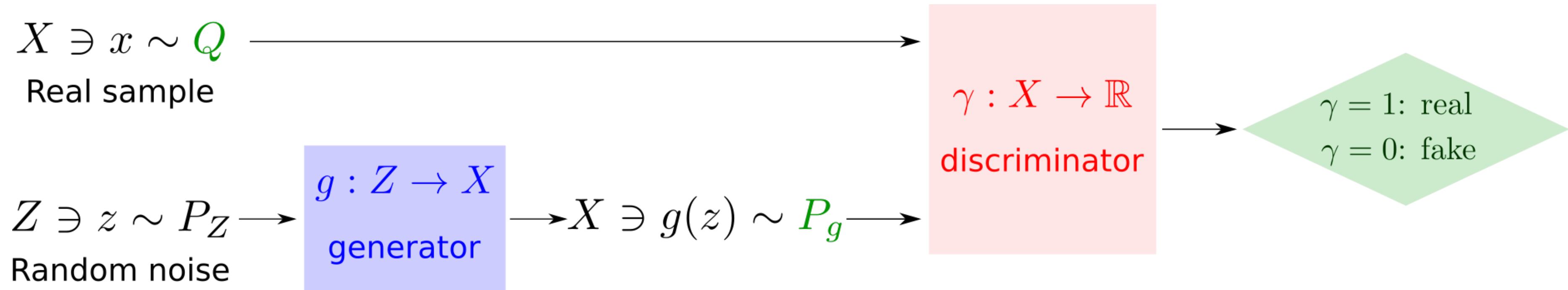


$$\min_{g \in G} D^\Gamma(Q \| P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g), \quad \underline{Q \text{ is } \Sigma\text{-invariant}}$$

- Target distribution Q is invariant under a group Σ .

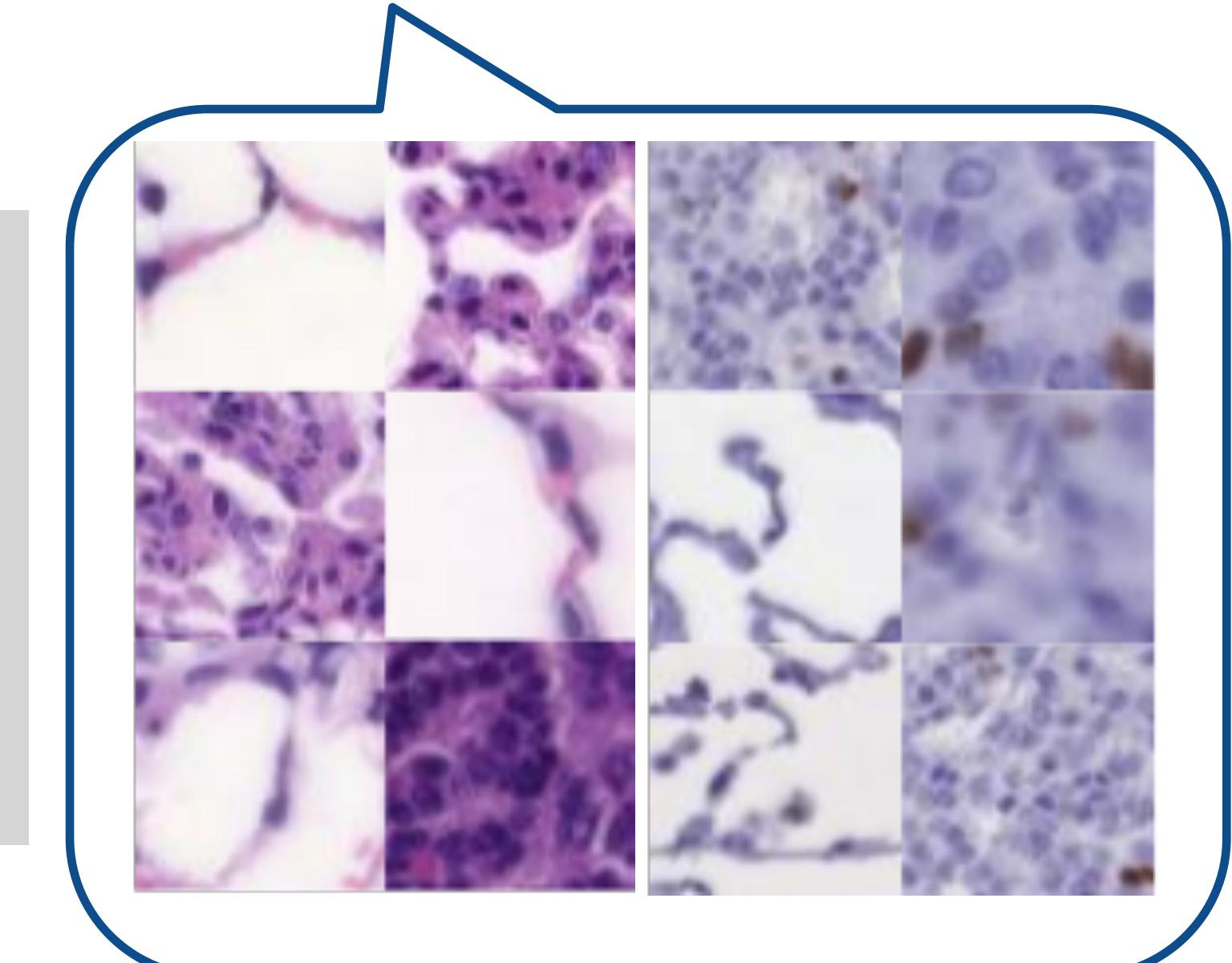


GAN with embedded structure

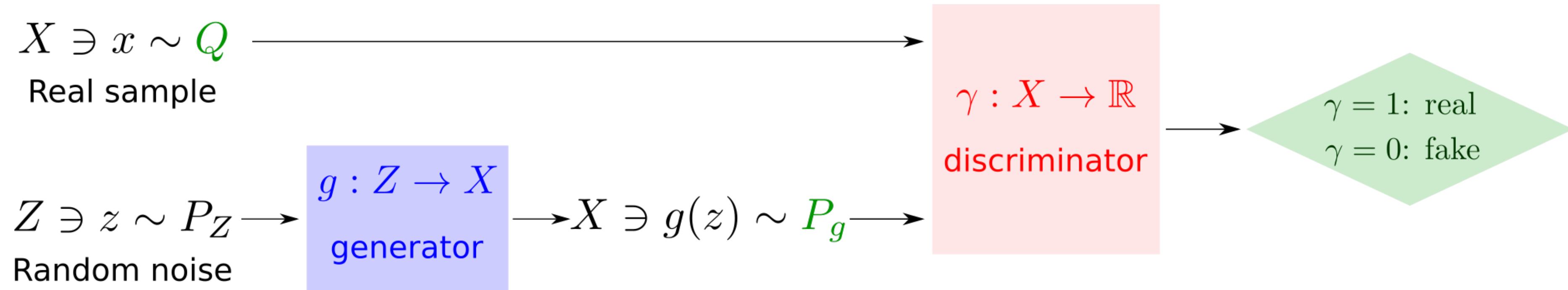


$$\min_{g \in G} D^\Gamma(Q \| P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g), \quad \underline{Q \text{ is } \Sigma\text{-invariant}}$$

- Target distribution Q is invariant under a group Σ .
- Σ : rotation, reflection, permutation, etc.

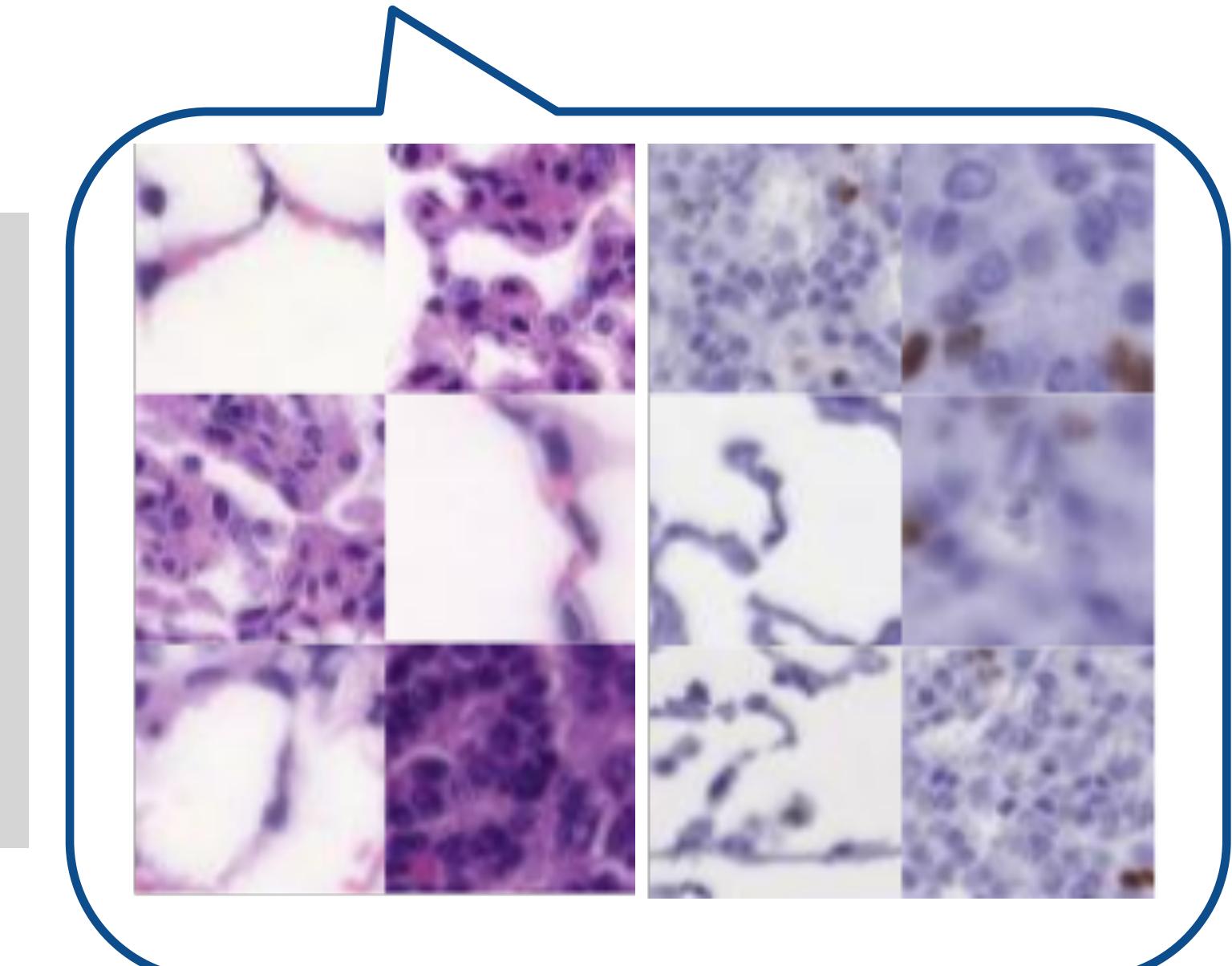


GAN with embedded structure



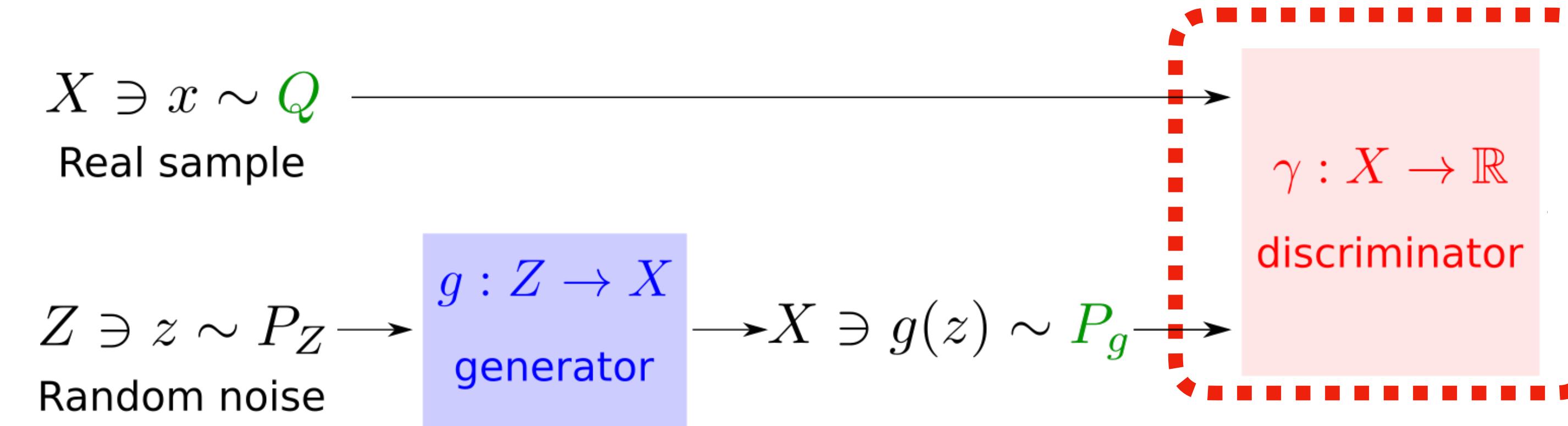
$$\min_{g \in G} D^\Gamma(Q \| P_g) = \min_{g \in G} \max_{\gamma \in \Gamma} H(\gamma; Q, P_g), \quad \underline{Q \text{ is } \Sigma\text{-invariant}}$$

- Target distribution Q is invariant under a group Σ .
- Σ : rotation, reflection, permutation, etc.
- **How to incorporate structure into g and γ ?**

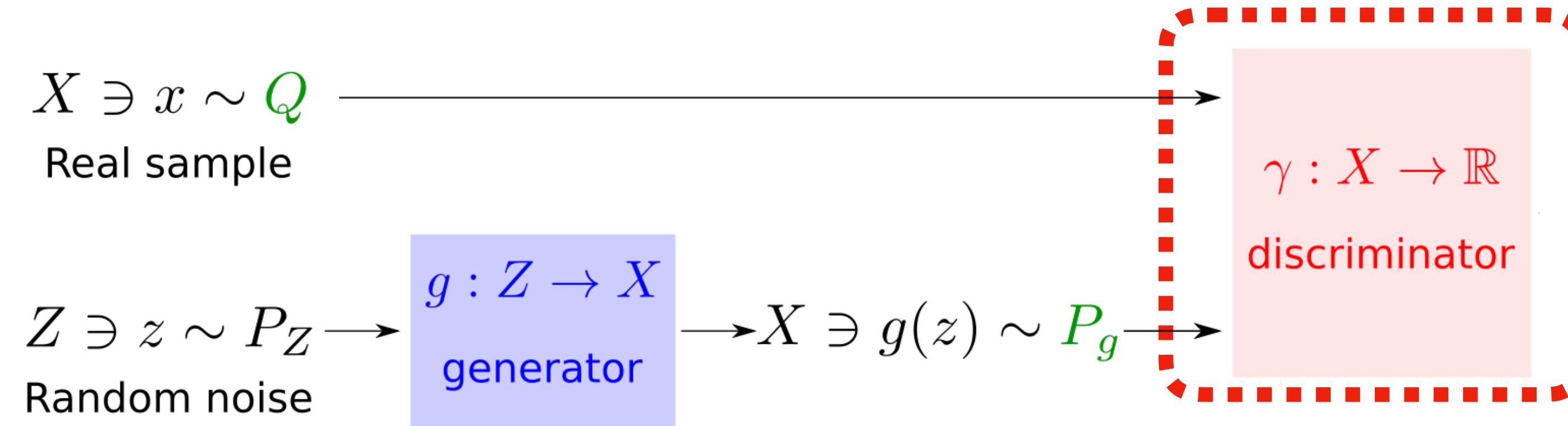


Theorem 1: “smarter” discriminator

Theorem 1: “smarter” discriminator



Theorem 1: “smarter” discriminator



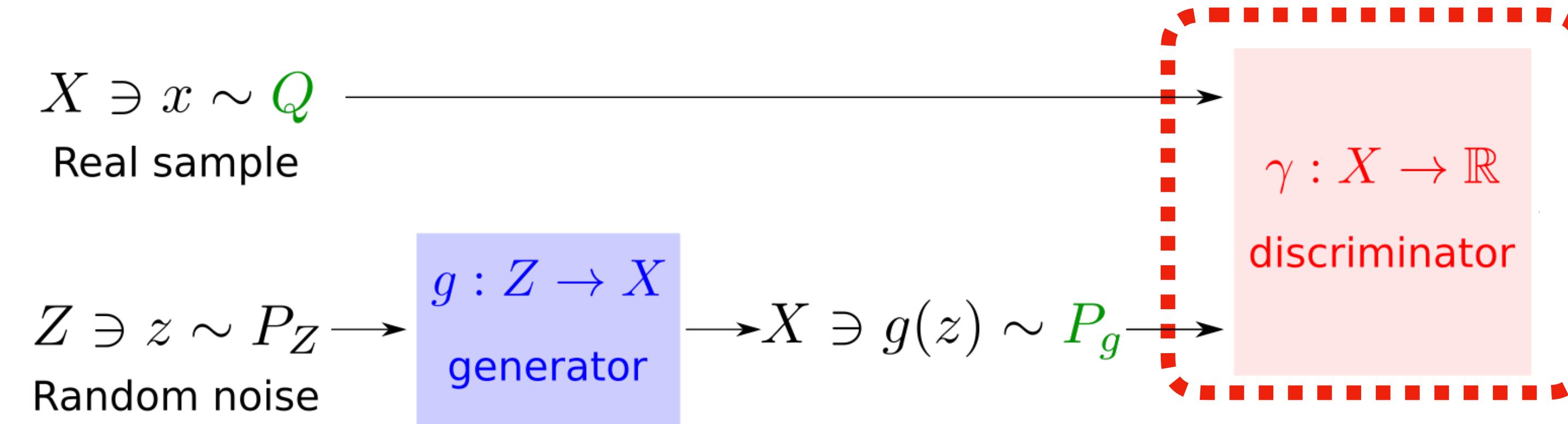
Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

Under mild assumptions on Σ and Γ , if the distributions P, Q are **Σ -invariant**, then

$$D^\Gamma(Q\|P) = D^{\Gamma_\Sigma^{\text{inv}}}(Q\|P) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} H(\gamma; Q, P),$$

- $\Gamma_\Sigma^{\text{inv}} \subset \Gamma$ is the subset of **Σ -invariant “smarter” discriminators**

Theorem 1: “smarter” discriminator



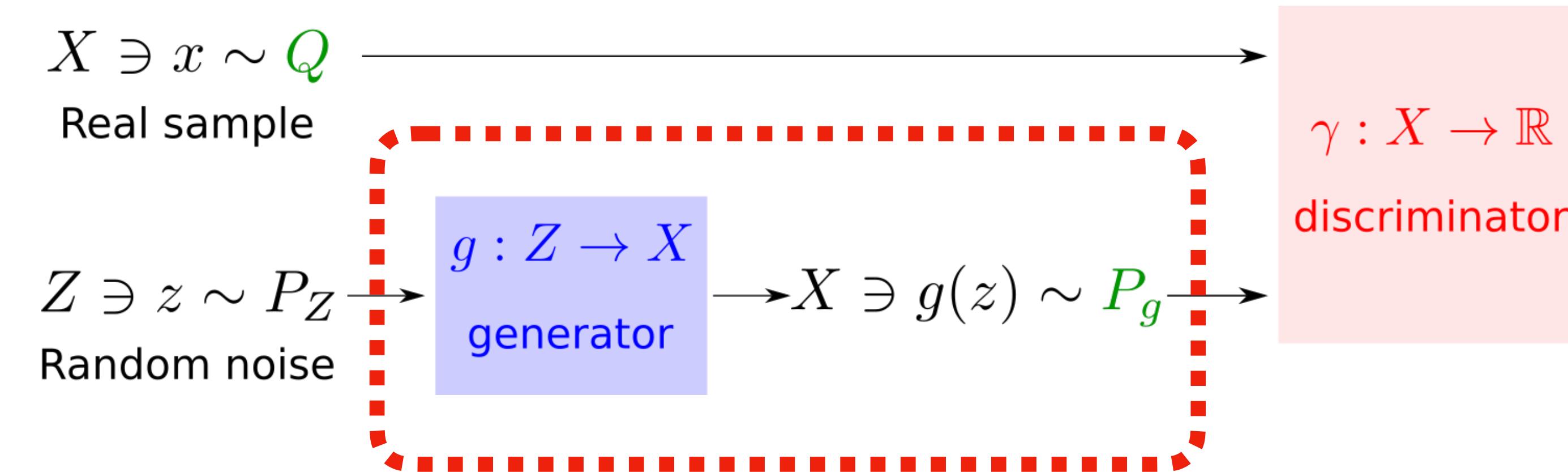
Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

Under mild assumptions on Σ and Γ , if the distributions P, Q are **Σ -invariant**, then

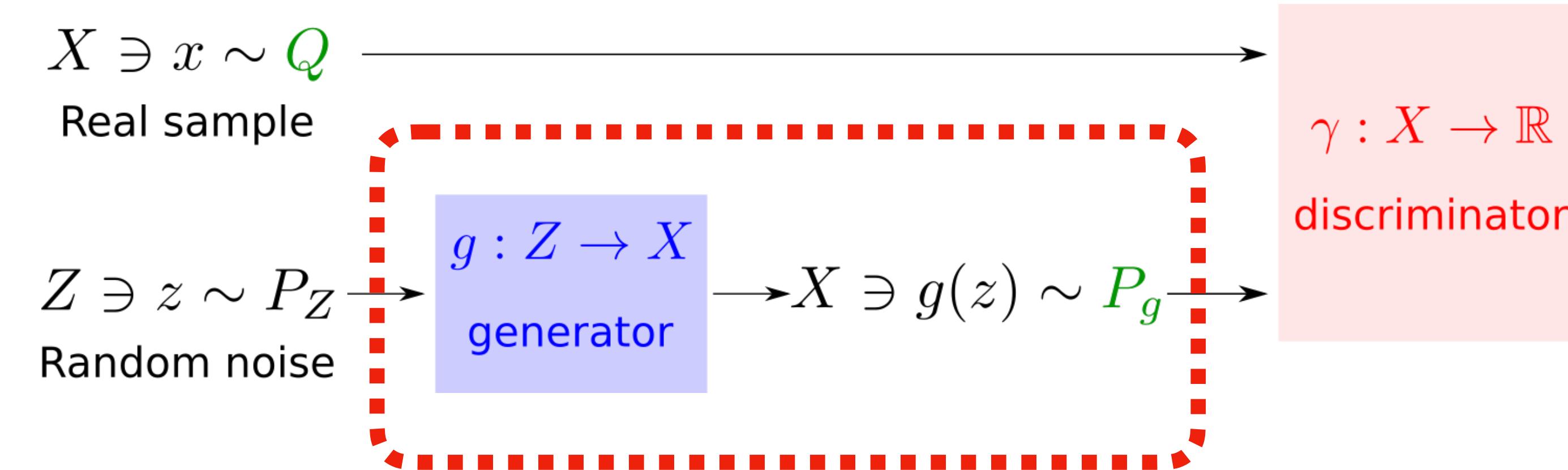
$$D^\Gamma(Q||P) = D^{\Gamma_\Sigma^{\text{inv}}}(Q||P) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} H(\gamma; Q, P),$$

- $\Gamma_\Sigma^{\text{inv}} \subset \Gamma$ is the subset of **Σ -invariant “smarter” discriminators**
- $\Gamma_\Sigma^{\text{inv}}$ serves as an **unbiased regularization** to prevent **discriminator overfitting**.

Theorem 2: “smarter” generator



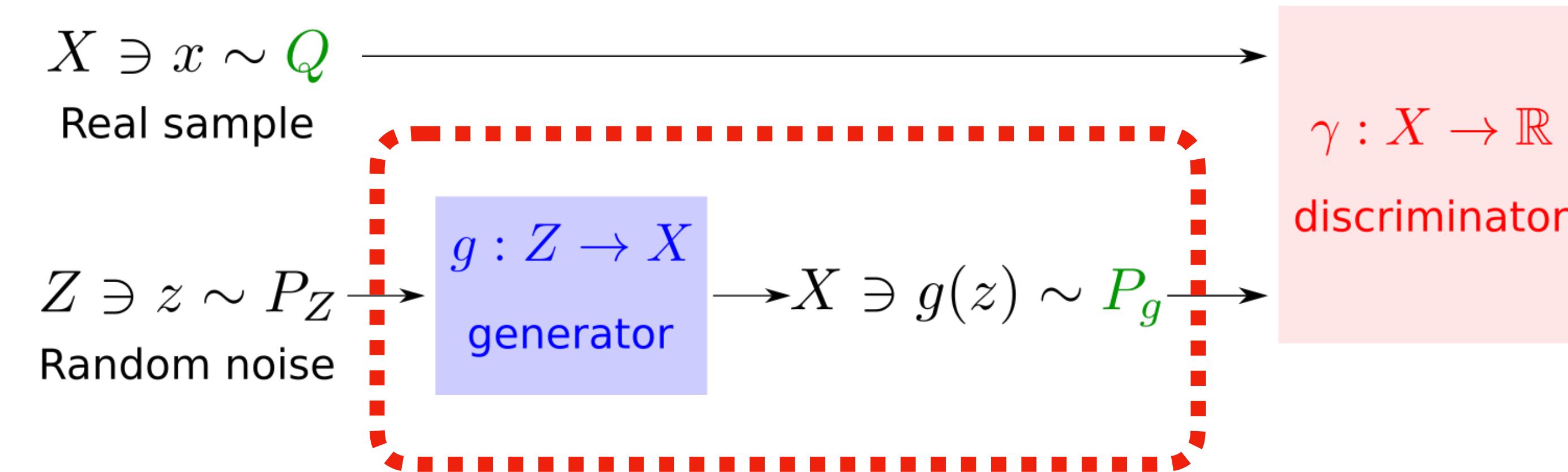
Theorem 2: “smarter” generator



Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

If P_Z is Σ -invariant and $g : Z \rightarrow X$ is Σ -equivariant, the generated measure P_g is Σ -invariant.

Theorem 2: “smarter” generator

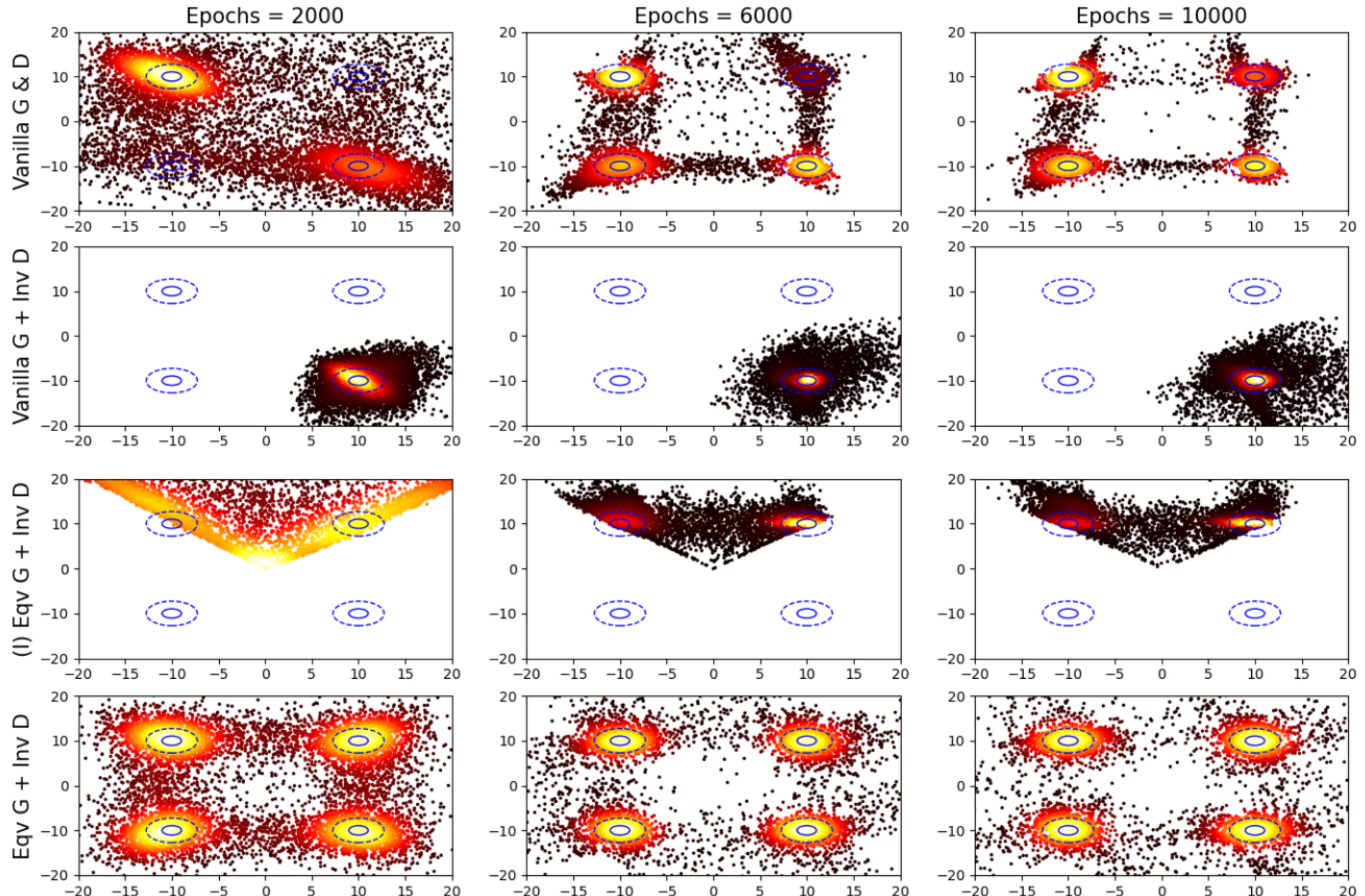


Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

If P_Z is Σ -invariant and $g : Z \rightarrow X$ is Σ -equivariant, the generated measure P_g is Σ -invariant.

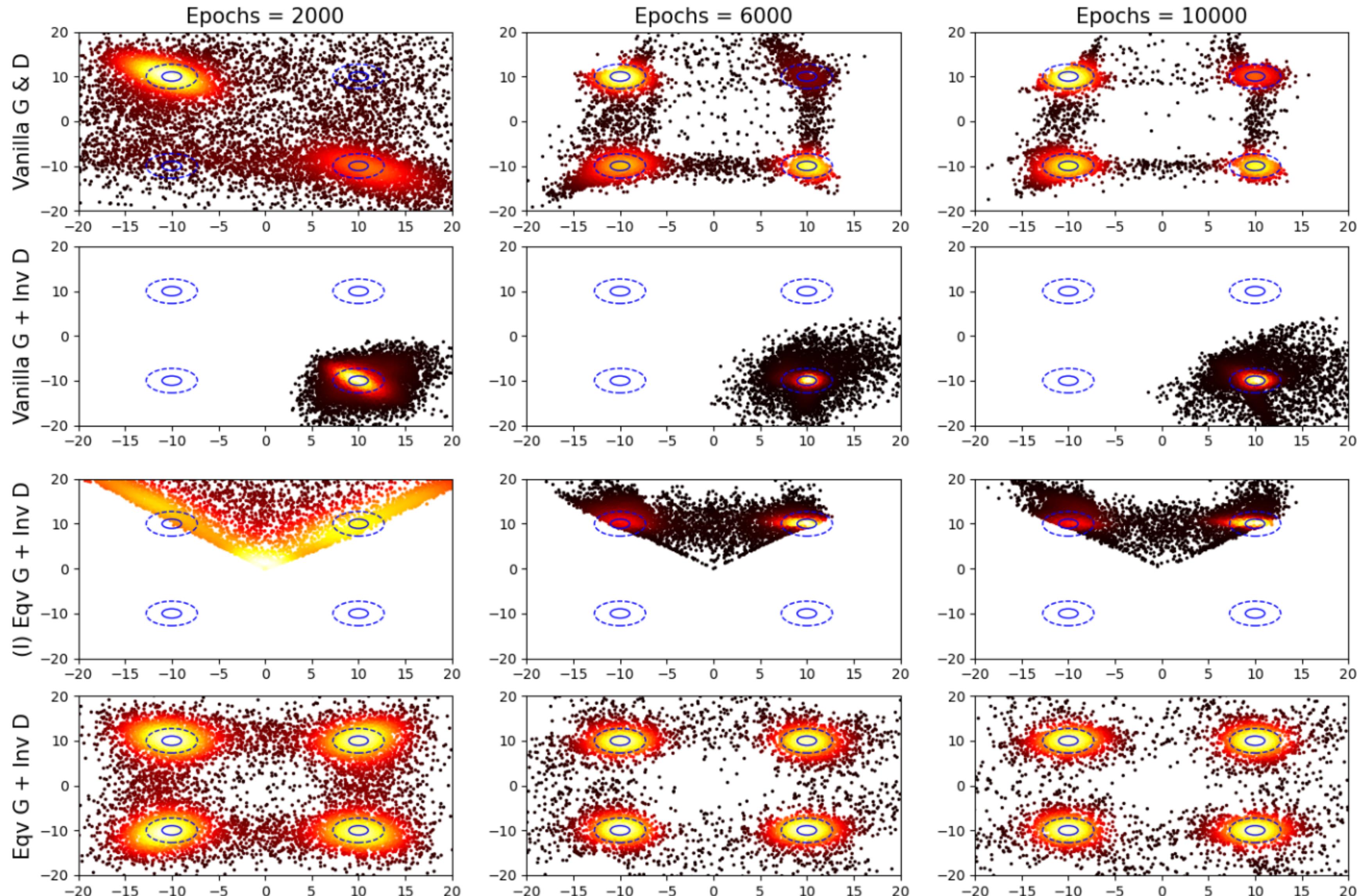
- Structure information embedded in the “smarter” generator **and noise source**.

Two “smart” players



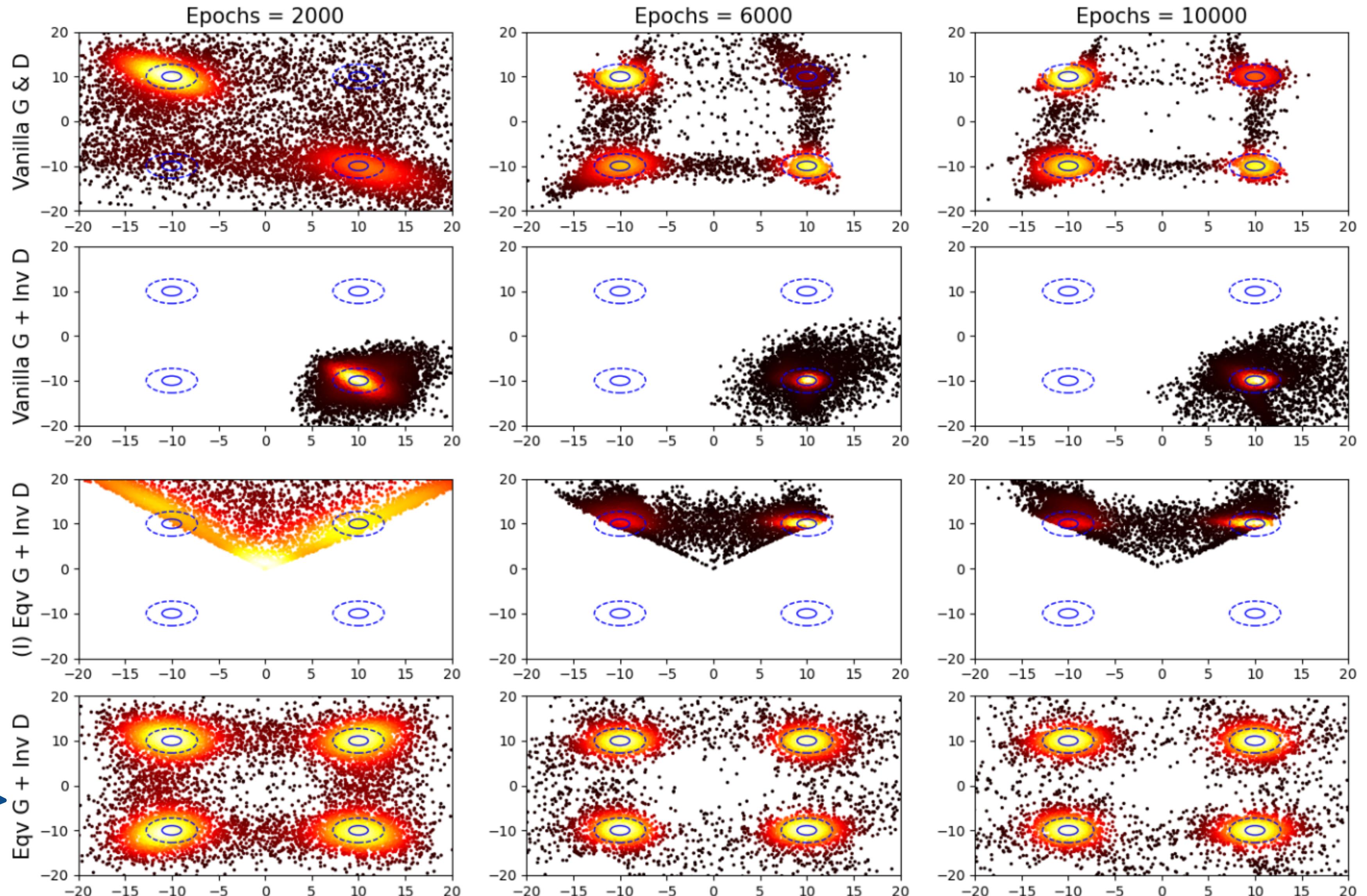
Two “smart” players

“Ignorant”
players need lots of
data, lots of time...
(the usual GANs)



Two “smart” players

“Ignorant”
players need lots of
data, lots of time...
(the usual GANs)



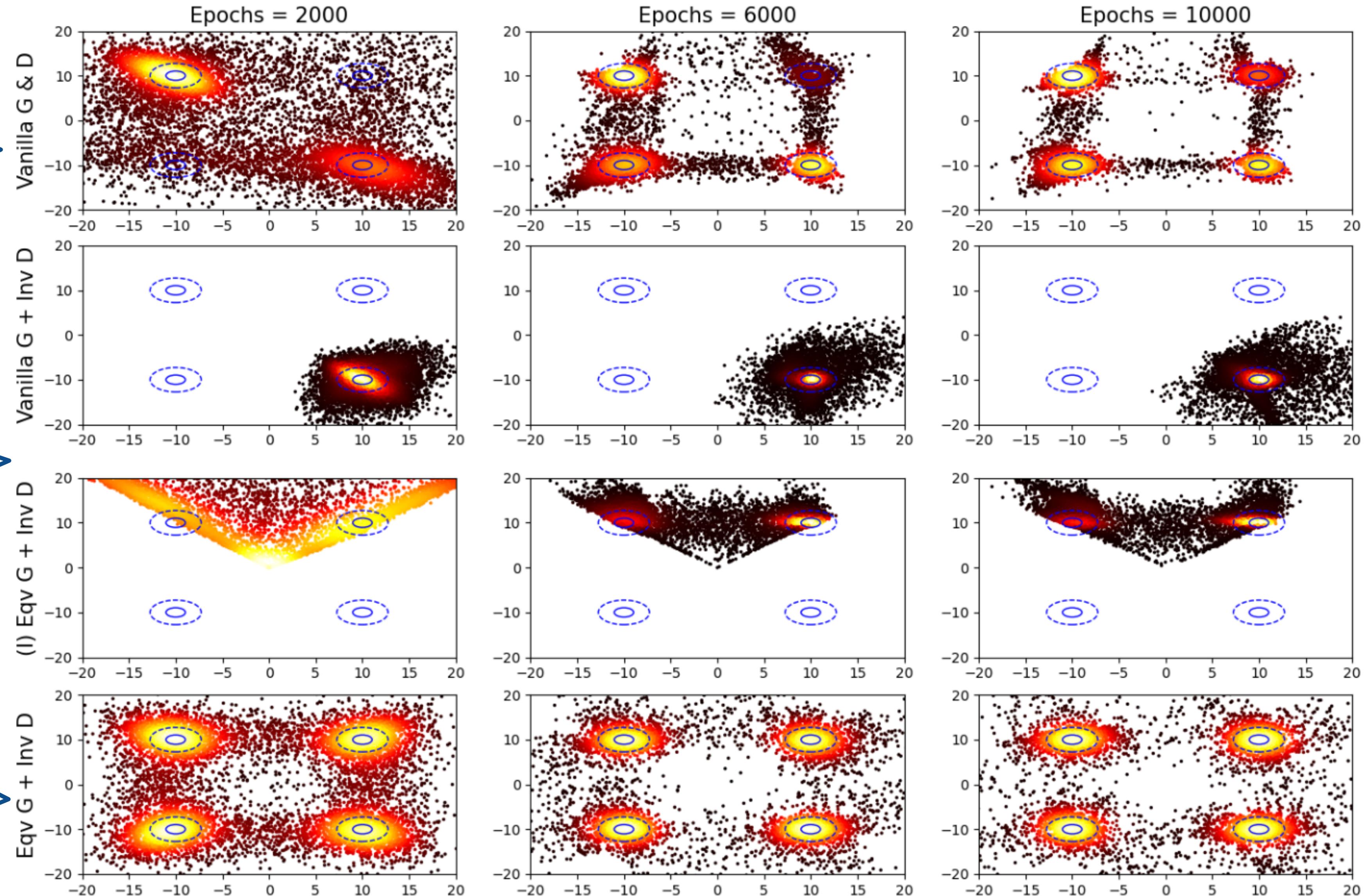
“Smart” players
learn faster and better
(our GANs)

Two “smart” players

“Ignorant”
players need lots of
data, lots of time...
(the usual GANs)

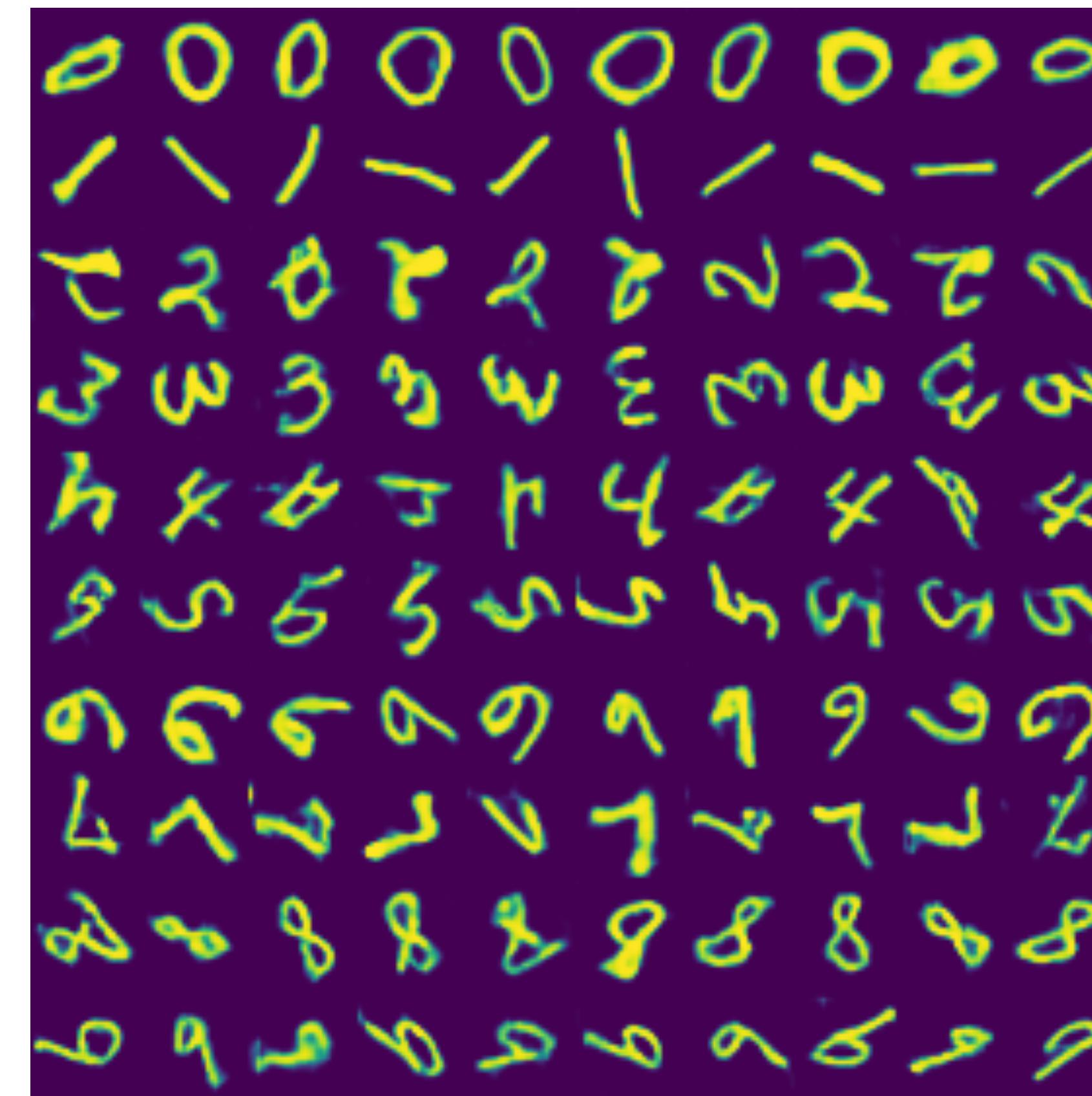
Players need to be
“equally smart”: no
weak links!

“Smart” players
learn faster and better
(our GANs)



RotMNIST with 1% training samples

“Ignorant” players

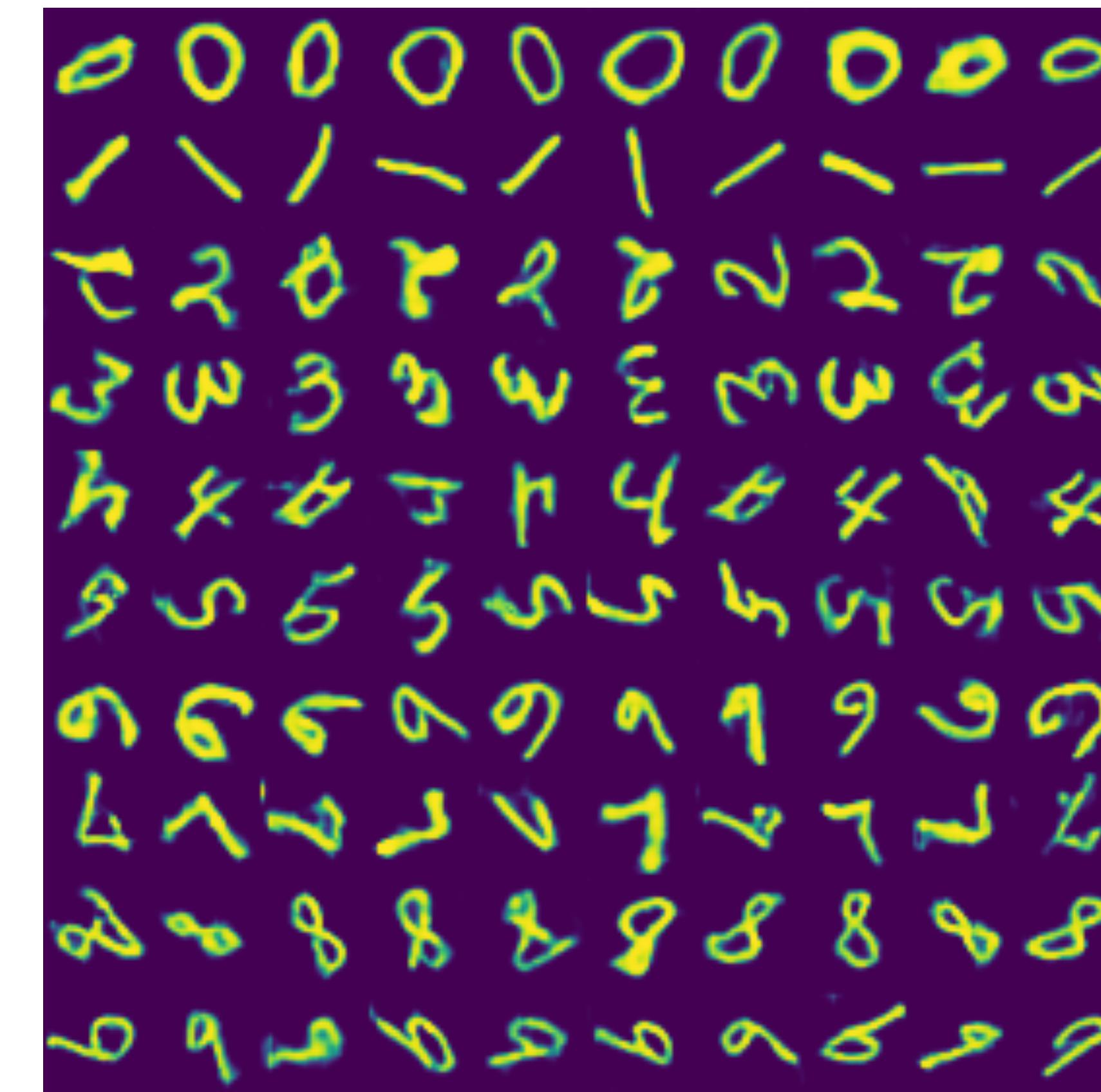


RotMNIST with 1% training samples

“Ignorant” players

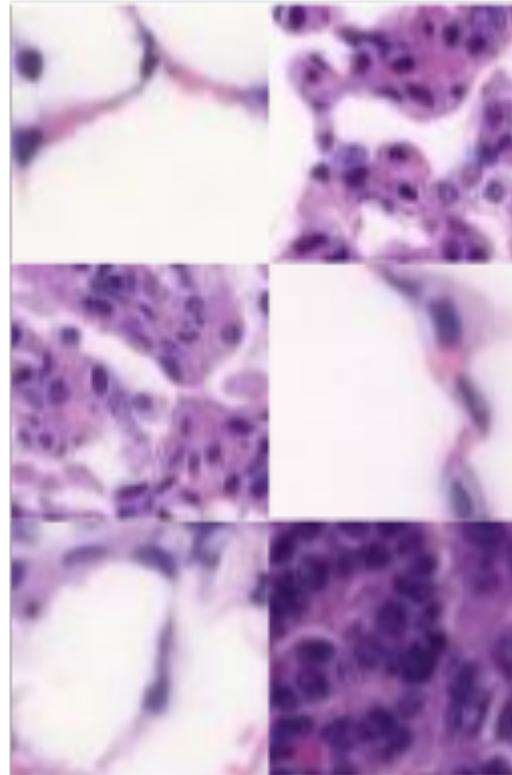
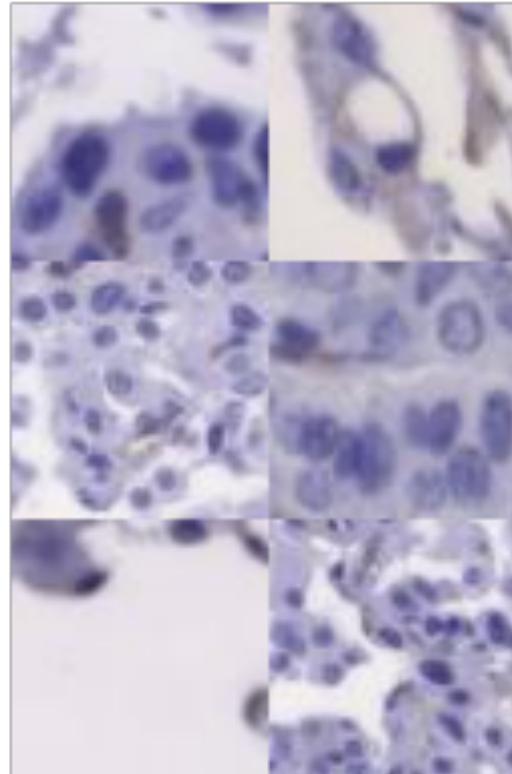


“Smart” players

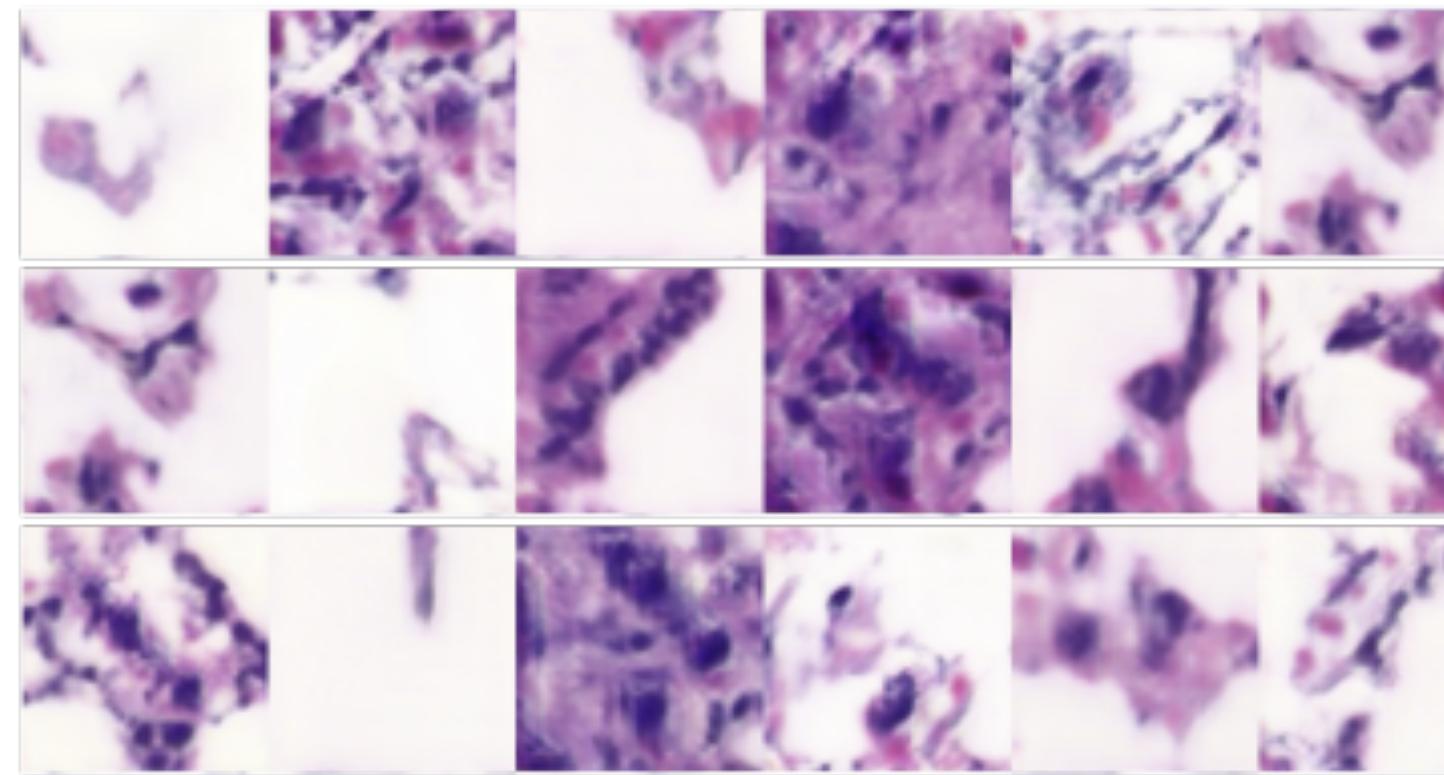
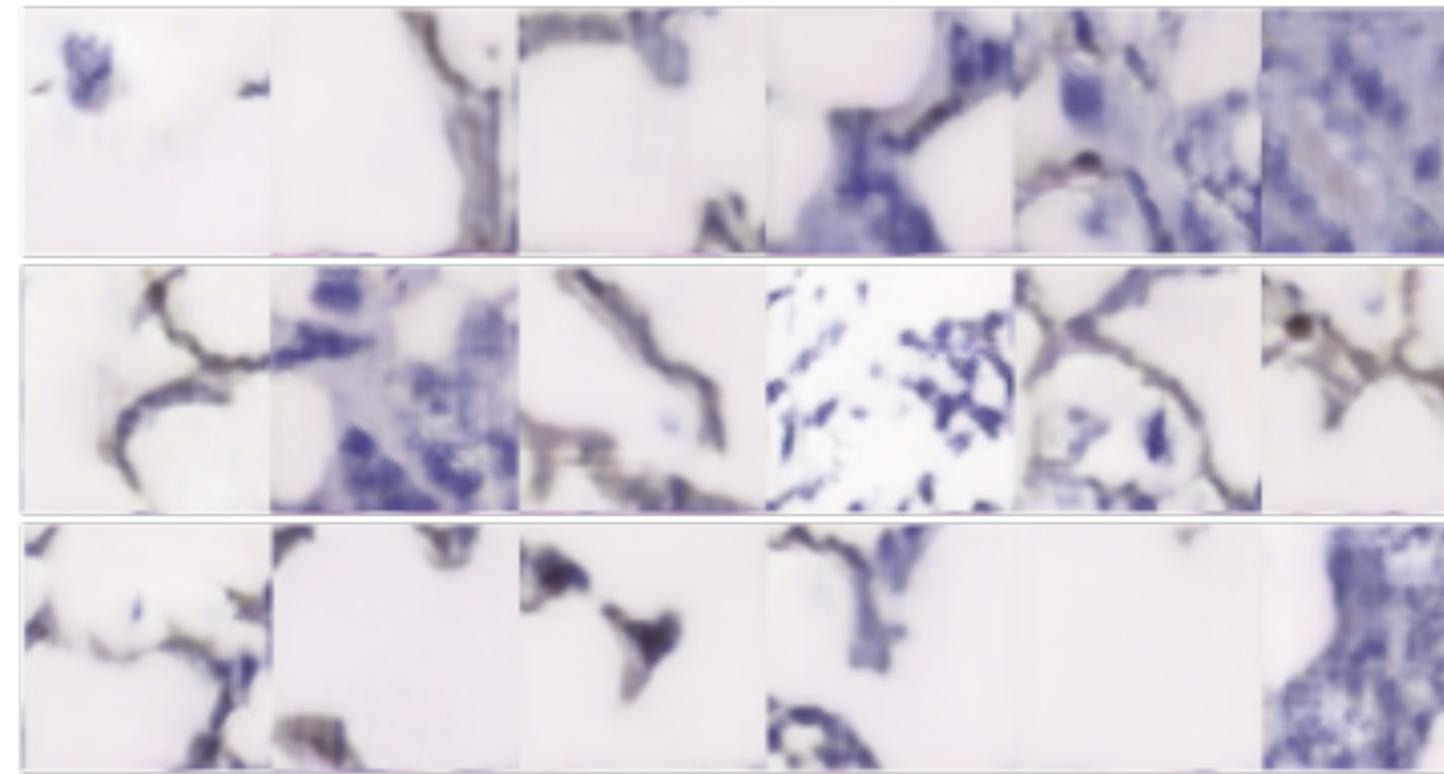


Medical images (ANHIR)

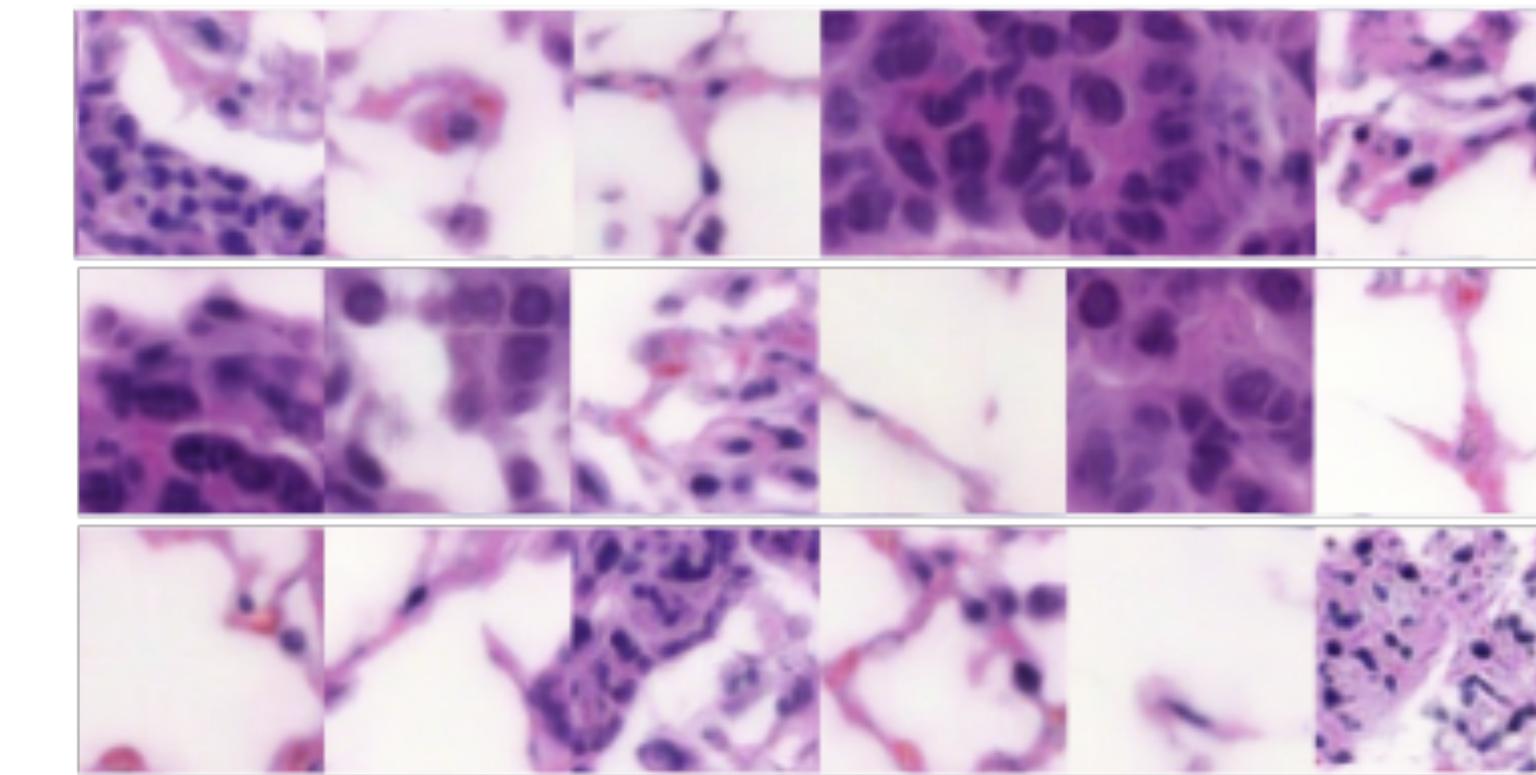
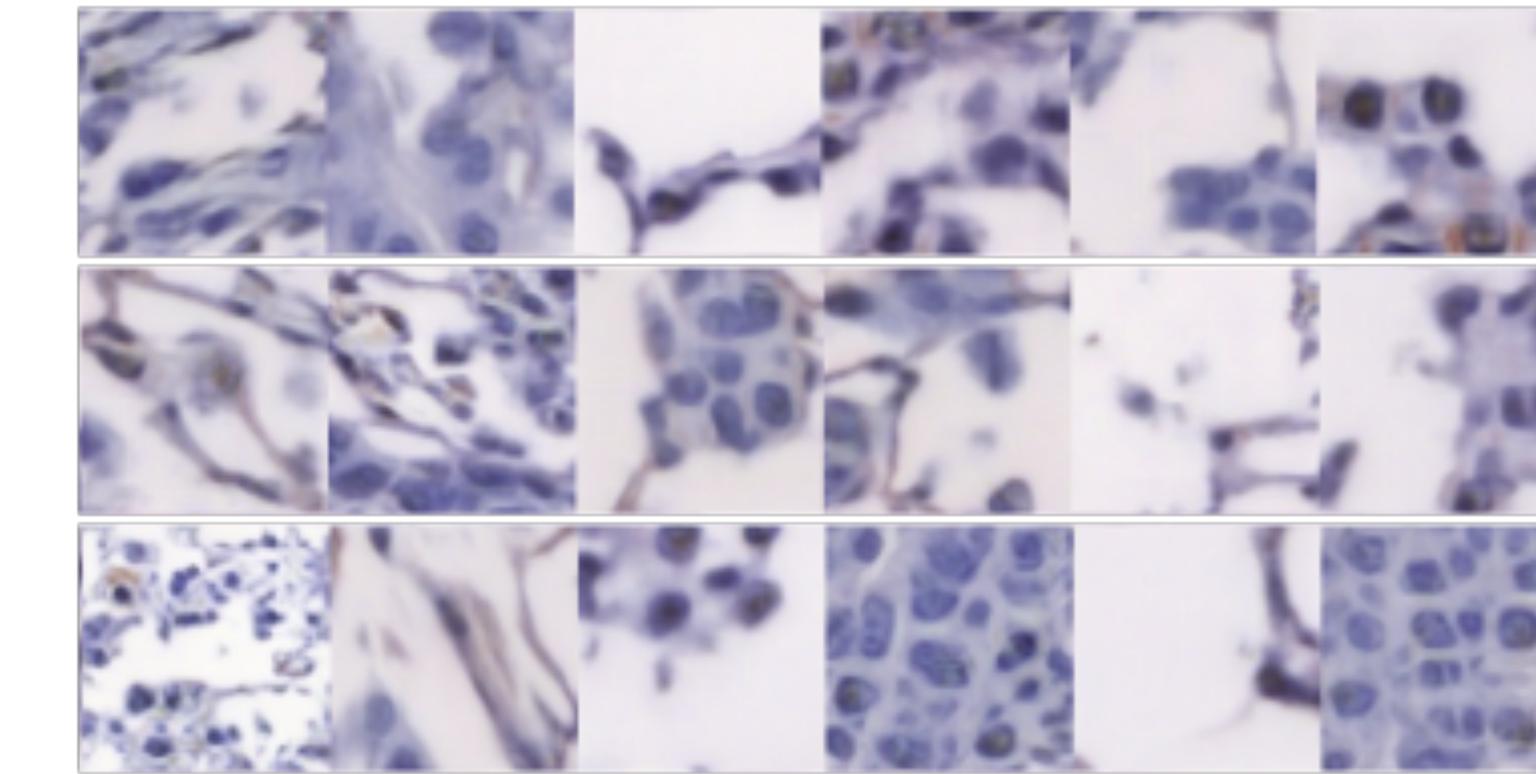
Real Samples



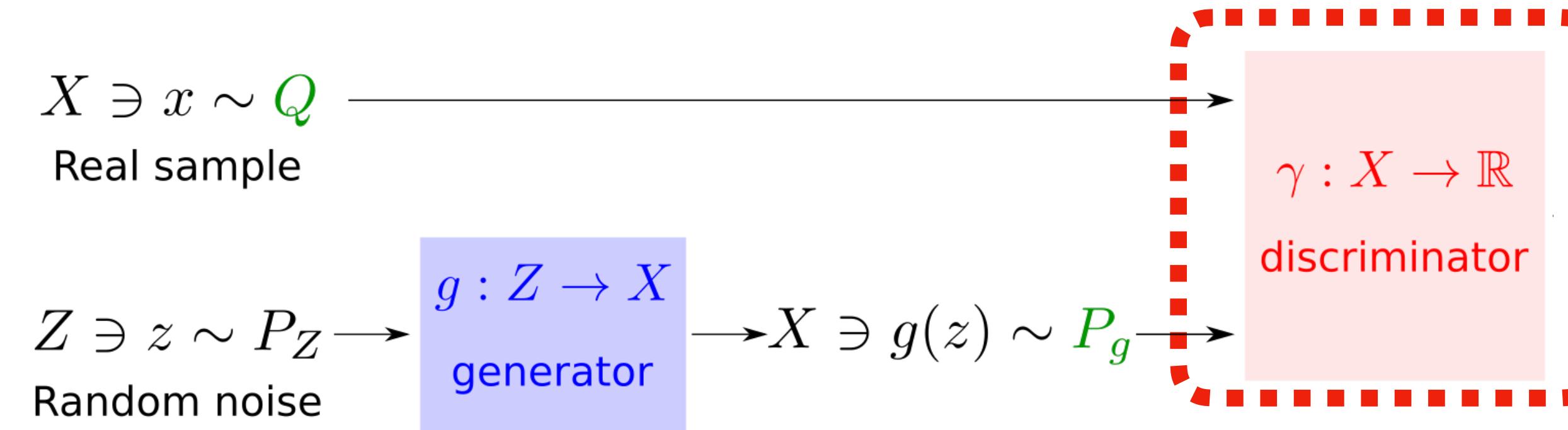
“Ignorant”
players



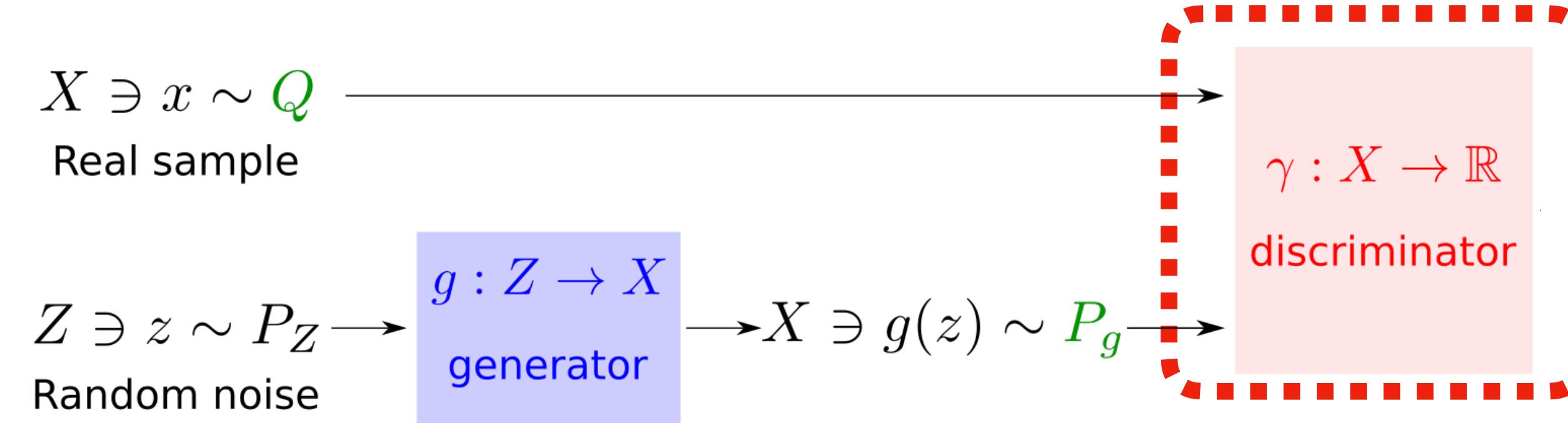
“Smart” players



What is the reason behind the improvement?



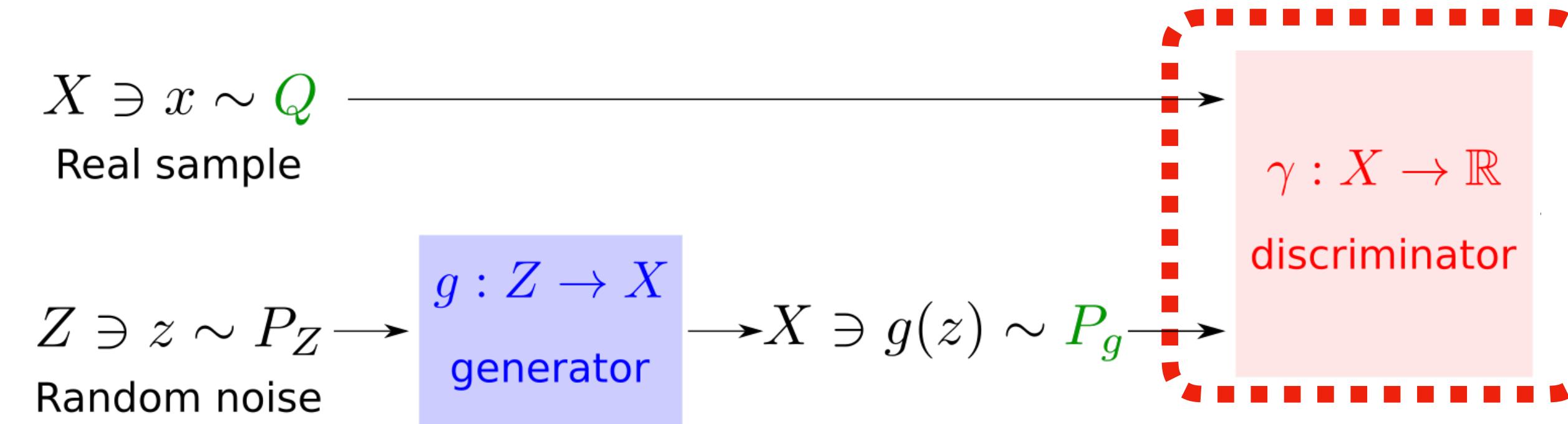
What is the reason behind the improvement?



P, Q are **Σ -invariant** $\implies D^{\Gamma}(Q\|P) = D^{\Gamma_{\Sigma}^{\text{inv}}}(Q\|P)$,

- Reducing Γ to $\Gamma_{\Sigma}^{\text{inv}}$ provides a better **empirical estimation** for $D^{\Gamma}(Q\|P)$.

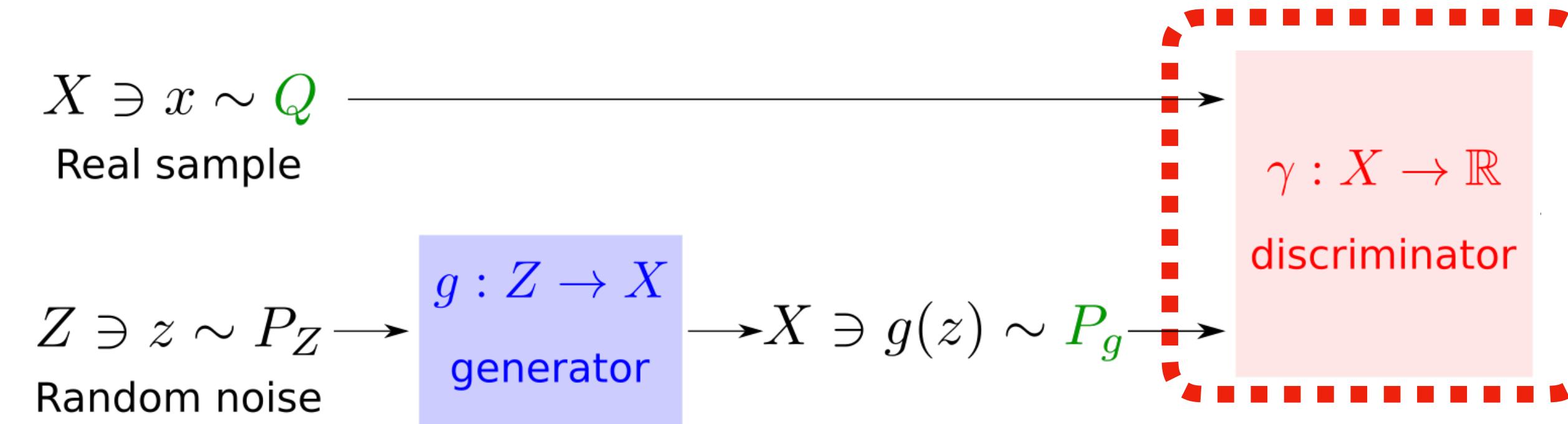
What is the reason behind the improvement?



P, Q are **Σ -invariant** $\implies D^\Gamma(Q||P) = D^{\Gamma_\Sigma^{\text{inv}}}(Q||P)$,

- Reducing Γ to $\Gamma_\Sigma^{\text{inv}}$ provides a better **empirical estimation** for $D^\Gamma(Q||P)$.
- $(x_1, \dots, x_m) \sim P, (y_1, \dots, y_n) \sim Q \implies \text{Empirical measures } P_m = \frac{1}{m} \sum_{i=1}^m \delta_{x_i}, Q_n = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$

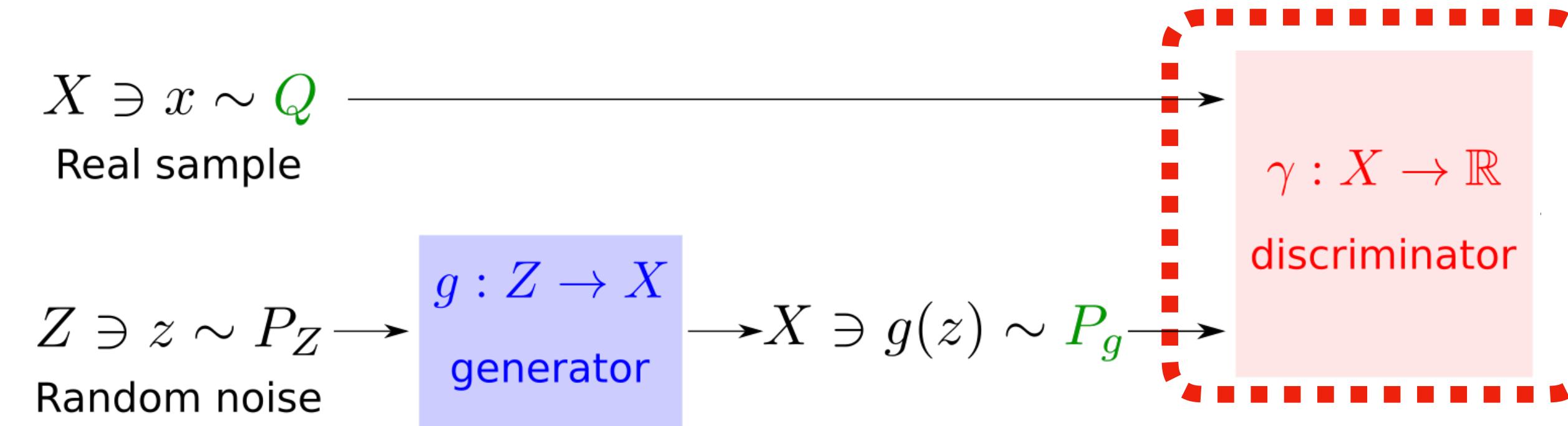
What is the reason behind the improvement?



P, Q are **Σ -invariant** $\implies D^\Gamma(Q||P) = D^{\Gamma_\Sigma^{\text{inv}}}(Q||P)$,

- Reducing Γ to $\Gamma_\Sigma^{\text{inv}}$ provides a better **empirical estimation** for $D^\Gamma(Q||P)$.
- $(x_1, \dots, x_m) \sim P, (y_1, \dots, y_n) \sim Q \implies \text{Empirical measures } P_m = \frac{1}{m} \sum_{i=1}^m \delta_{x_i}, Q_n = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$
- $D^\Gamma(Q||P) \approx \cancel{D^\Gamma(\cancel{Q_n}||\cancel{P_m})} = D^{\Gamma_\Sigma^{\text{inv}}}(Q_n||P_m)$

What is the reason behind the improvement?



P, Q are **Σ -invariant** $\implies D^\Gamma(Q||P) = D^{\Gamma_\Sigma^{\text{inv}}}(Q||P)$,

- Reducing Γ to $\Gamma_\Sigma^{\text{inv}}$ provides a better **empirical estimation** for $D^\Gamma(Q||P)$.
- $(x_1, \dots, x_m) \sim P, (y_1, \dots, y_n) \sim Q \implies \text{Empirical measures } P_m = \frac{1}{m} \sum_{i=1}^m \delta_{x_i}, Q_n = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$
- $D^\Gamma(Q||P) \approx \cancel{D^\Gamma(\cancel{Q_n}||\cancel{P_m})} = D^{\Gamma_\Sigma^{\text{inv}}}(Q_n||P_m)$

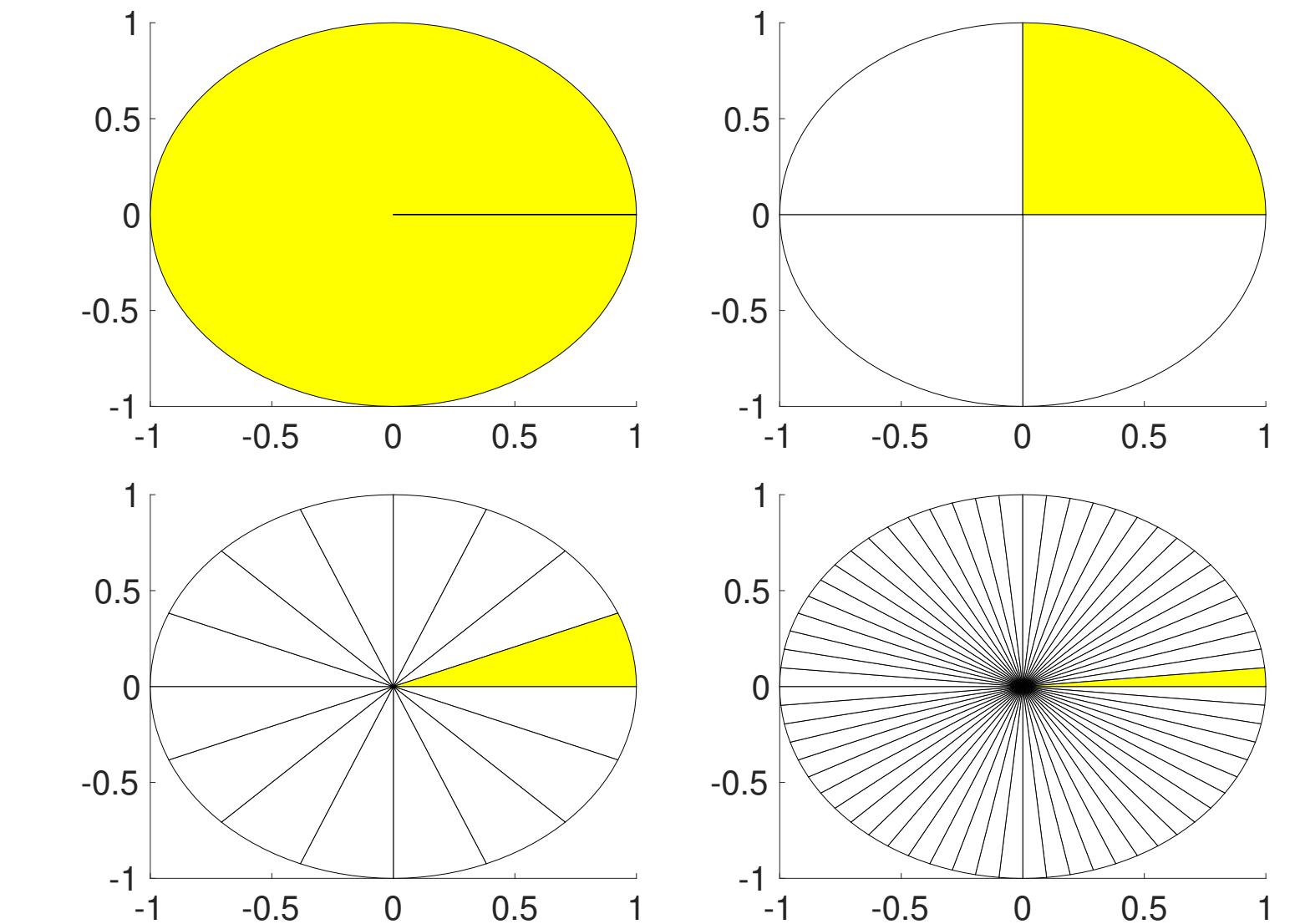
Question: How much **more accurate** is the new estimation?

Wasserstein-1 metric

- $W(Q, P) = \sup_{\gamma \in \Gamma} \{ \mathbb{E}_Q[\gamma] - \mathbb{E}_P[\gamma] \}$. $\Gamma = \text{Lip}_1(X)$
- **Estimator:** $W^\Sigma(Q_n, P_m) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} \{ \mathbb{E}_{Q_n}[\gamma] - \mathbb{E}_{P_m}[\gamma] \}$

Wasserstein-1 metric

- $W(Q, P) = \sup_{\gamma \in \Gamma} \{ \mathbb{E}_Q[\gamma] - \mathbb{E}_P[\gamma] \}$. $\Gamma = \text{Lip}_1(X)$
- **Estimator:** $W^\Sigma(Q_n, P_m) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} \{ \mathbb{E}_{Q_n}[\gamma] - \mathbb{E}_{P_m}[\gamma] \}$



Theorem [Chen, Katsoulakis, Rey-Bellet, **Z.**, ICML 2023]

$X = \Sigma \times X_0$ bounded in \mathbb{R}^d , and $P, Q \in \mathcal{P}_\Sigma(X)$ are Σ -invariant. With high probability,

- when $d \geq 2$: $\forall s > 0, |W(Q, P) - W^\Sigma(Q_n, P_m)| \leq C \left(\left(\frac{1}{|\Sigma| m} \right)^{\frac{1}{d+s}} + \left(\frac{1}{|\Sigma| n} \right)^{\frac{1}{d+s}} \right)$
- when $d = 1$: $|W(Q, P) - W^\Sigma(Q_n, P_m)| \leq C \cdot \text{diam}(X_0) \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right)$

Maximum Mean Discrepancy (MMD)

- $\text{MMD}(Q, P) = \sup_{\gamma \in \Gamma} \{\mathbb{E}_Q[\gamma] - \mathbb{E}_P[\gamma]\}$. Γ is the unit ball in some **RKHS** \mathcal{H} with kernel $k(x, y)$.
- **Estimator:** $\text{MMD}^\Sigma(Q_n, P_m) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} \{\mathbb{E}_{Q_n}[\gamma] - \mathbb{E}_{P_m}[\gamma]\}$

Maximum Mean Discrepancy (MMD)

- $\text{MMD}(Q, P) = \sup_{\gamma \in \Gamma} \{\mathbb{E}_Q[\gamma] - \mathbb{E}_P[\gamma]\}$. Γ is the unit ball in some **RKHS** \mathcal{H} with kernel $k(x, y)$.
- **Estimator:** $\text{MMD}^\Sigma(Q_n, P_m) = \sup_{\gamma \in \Gamma_\Sigma^{\text{inv}}} \{\mathbb{E}_{Q_n}[\gamma] - \mathbb{E}_{P_m}[\gamma]\}$

Theorem [Chen, Katsoulakis, Rey-Bellet, Z., ICML 2023]

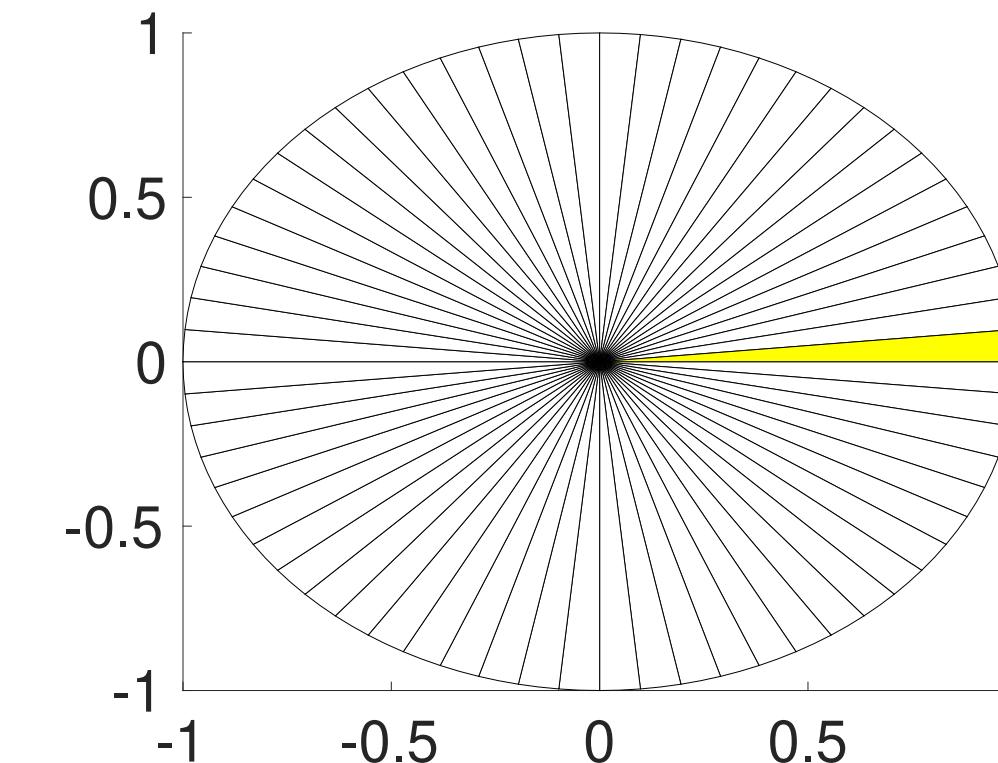
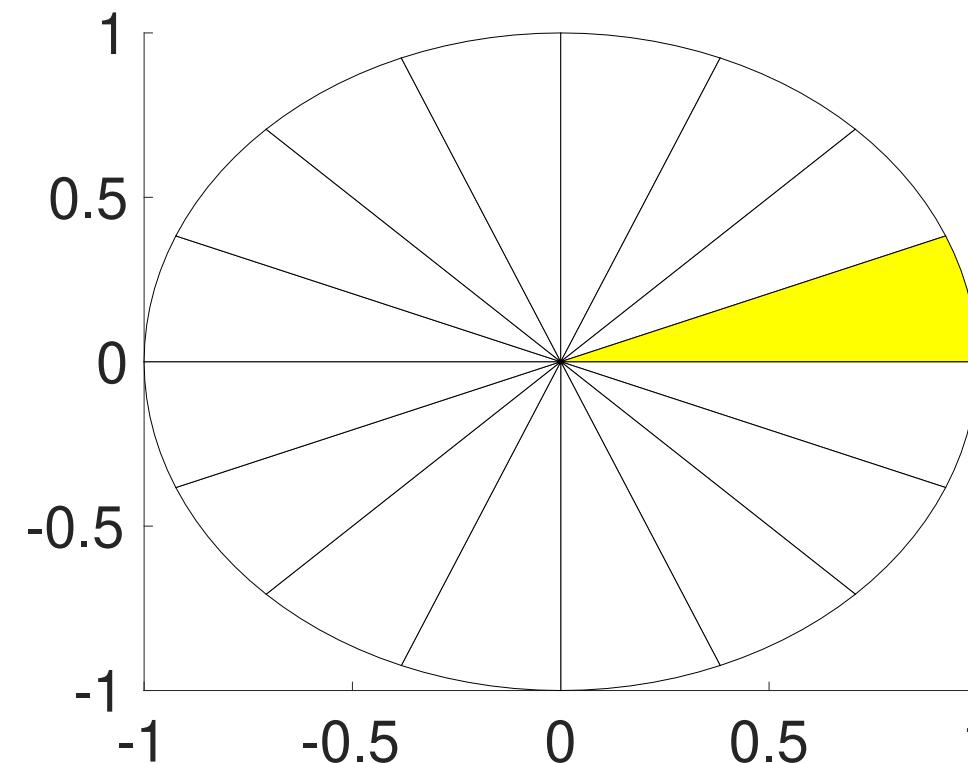
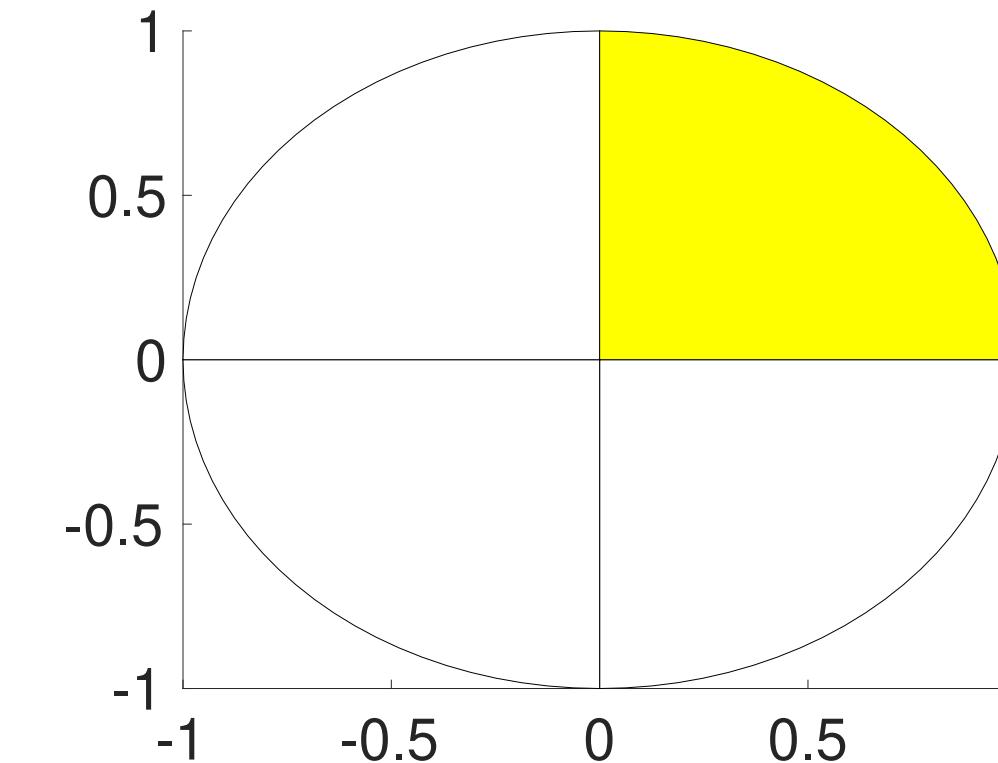
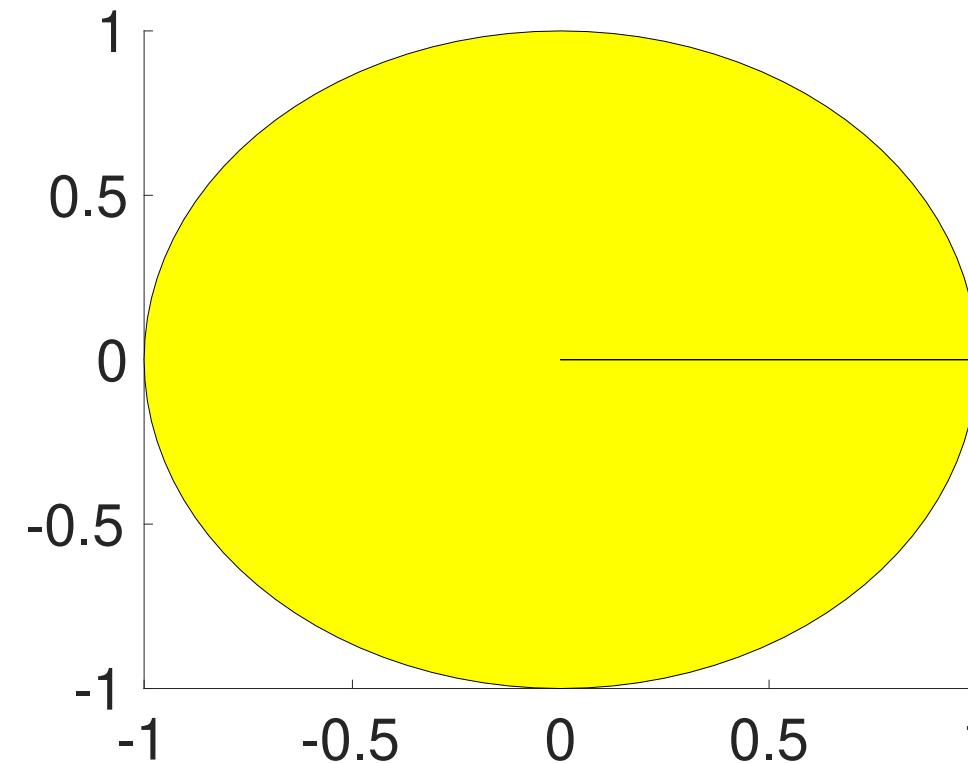
$X = \Sigma \times X_0$ bounded in \mathbb{R}^d , and $P, Q \in \mathcal{P}_\Sigma(X)$ are Σ -invariant. With high probability,

$$|\text{MMD}(Q, P) - \text{MMD}^\Sigma(Q_n, P_m)| = O\left(C_{\Sigma, k} \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right)\right),$$

where $C_{\Sigma, k} = \sqrt{a_{\Sigma, k} + \frac{1 - a_{\Sigma, k}}{|\Sigma|}}$, and $a_{\Sigma, k} \in (0, 1)$ depends on Σ and the **kernel** $k(x, y)$.

Maximum Mean Discrepancy (MMD)

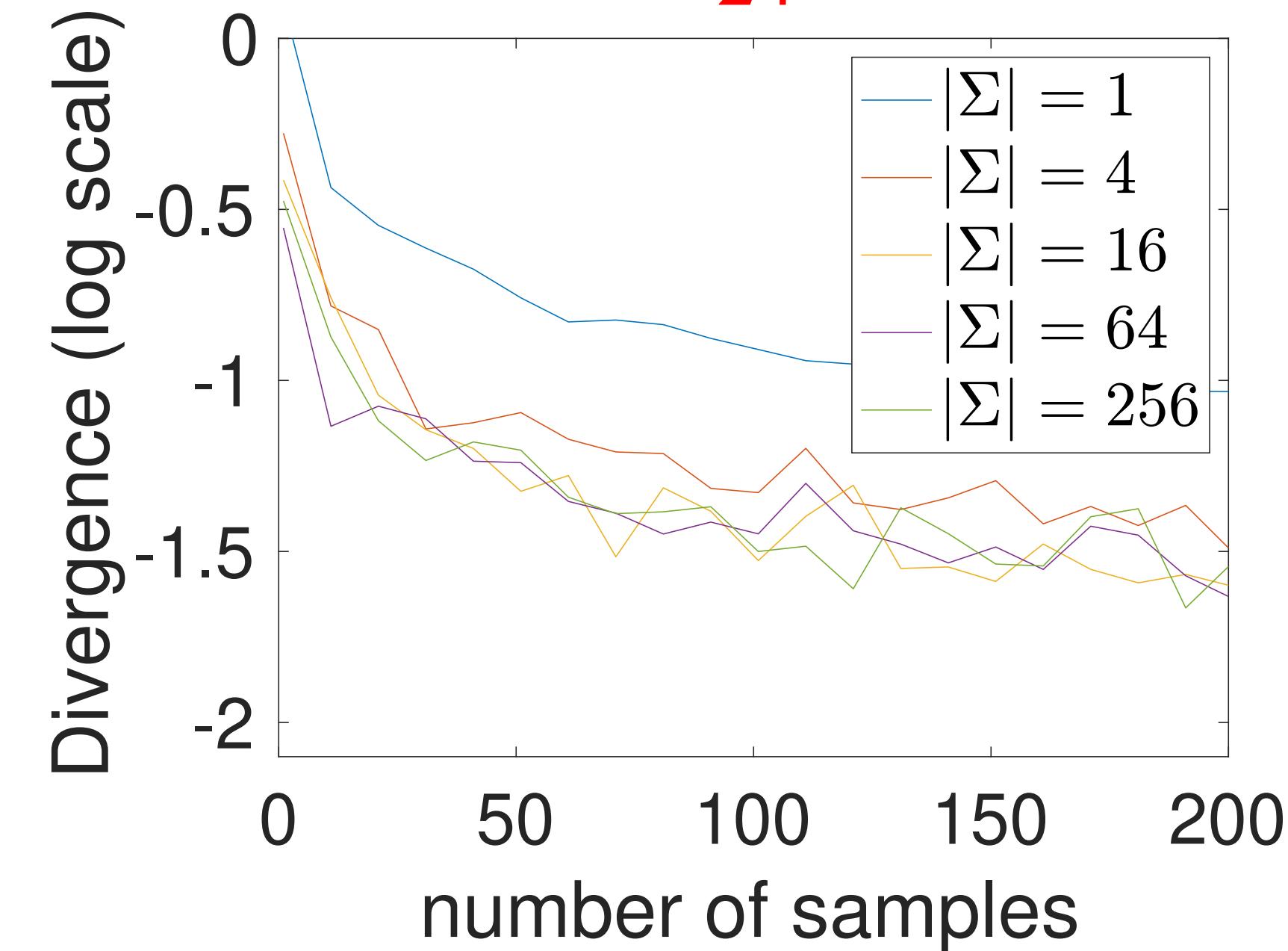
$$\left| \text{MMD}(Q, P) - \text{MMD}^{\Sigma}(Q_n, P_m) \right| = O\left(C_{\Sigma, k} \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right) \right), \quad C_{\Sigma, k} = \sqrt{a_{\Sigma, k} + \frac{1 - a_{\Sigma, k}}{|\Sigma|}}$$



Maximum Mean Discrepancy (MMD)

$$\left| \text{MMD}(\mathcal{Q}, \mathcal{P}) - \text{MMD}^{\Sigma}(\mathcal{Q}_n, \mathcal{P}_m) \right| = O \left(C_{\Sigma, k} \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right) \right), \quad C_{\Sigma, k} = \sqrt{a_{\Sigma, k} + \frac{1 - a_{\Sigma, k}}{|\Sigma|}}$$

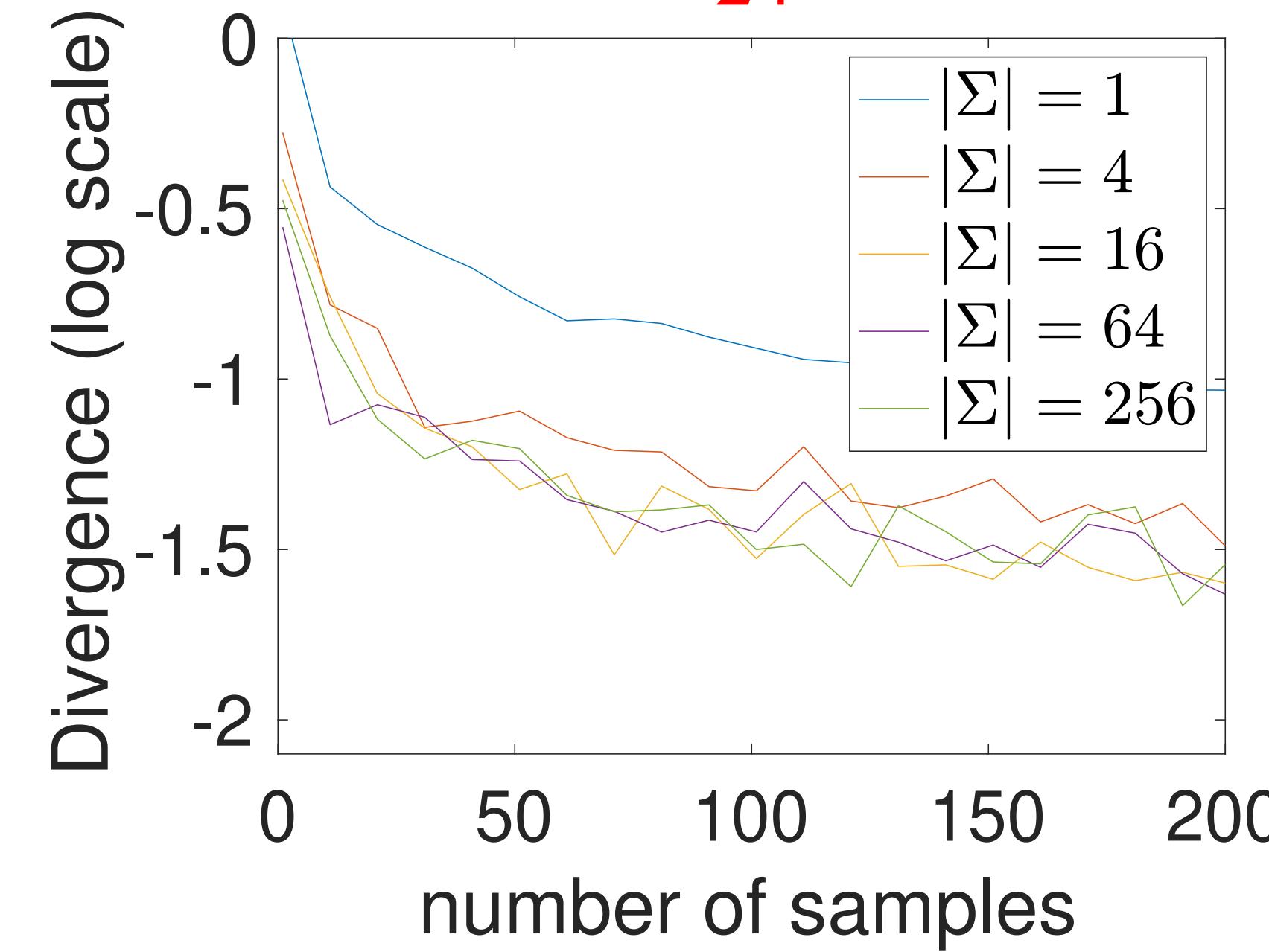
$$s = \frac{2\pi}{24}$$



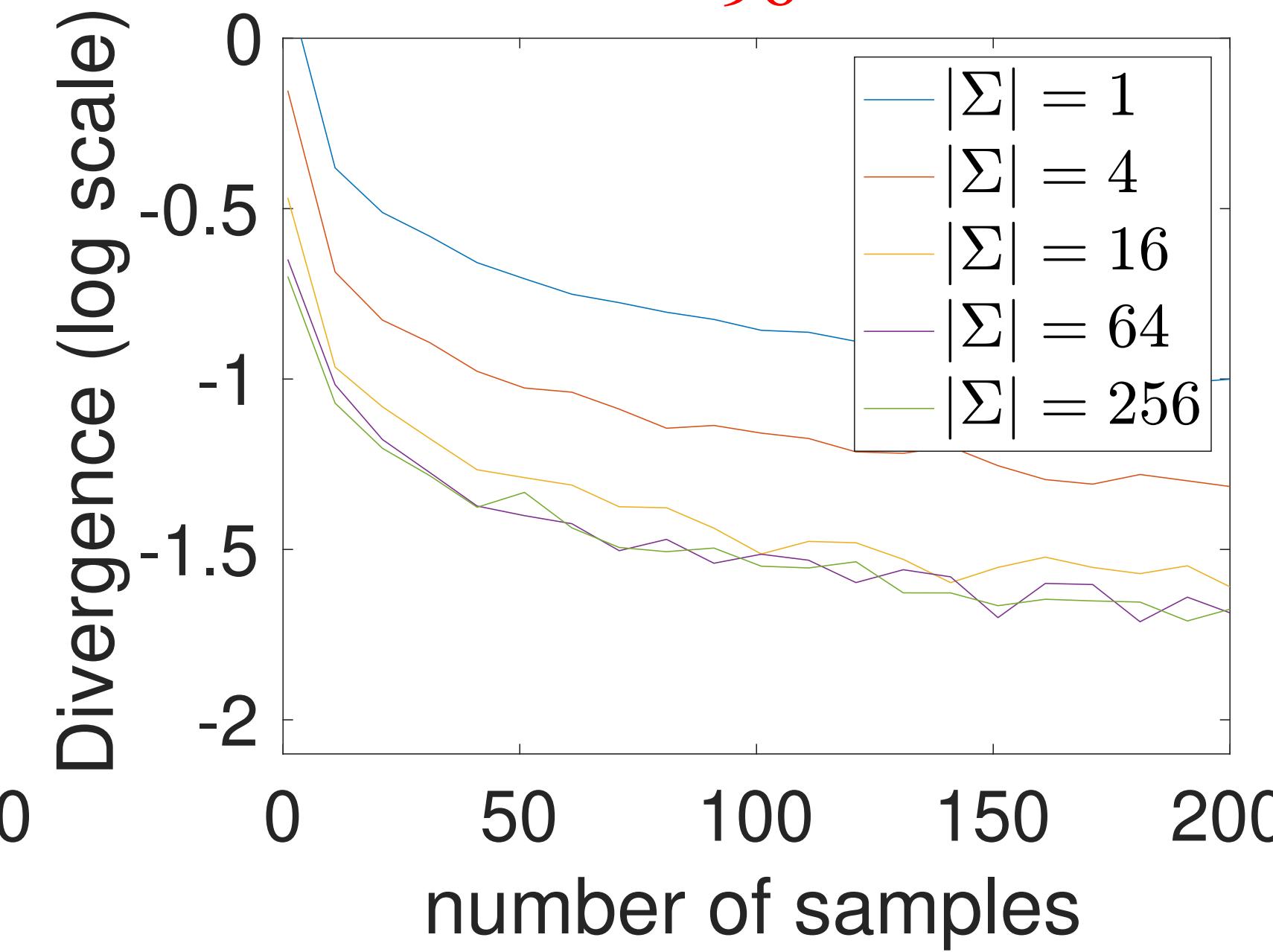
Maximum Mean Discrepancy (MMD)

$$\left| \text{MMD}(Q, P) - \text{MMD}^{\Sigma}(Q_n, P_m) \right| = O \left(C_{\Sigma, k} \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right) \right), \quad C_{\Sigma, k} = \sqrt{a_{\Sigma, k} + \frac{1 - a_{\Sigma, k}}{|\Sigma|}}$$

$$s = \frac{2\pi}{24}$$



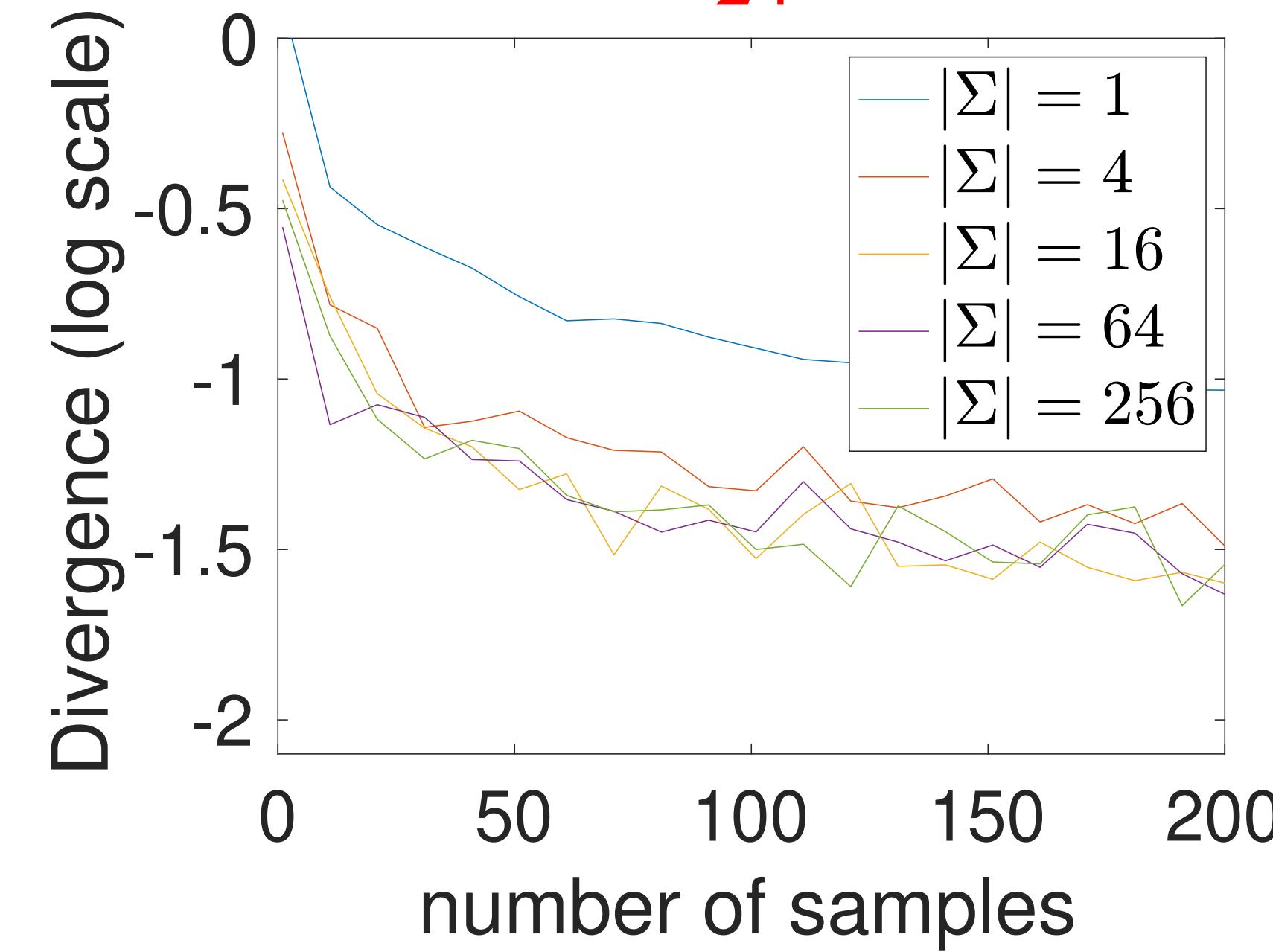
$$s = \frac{2\pi}{96}$$



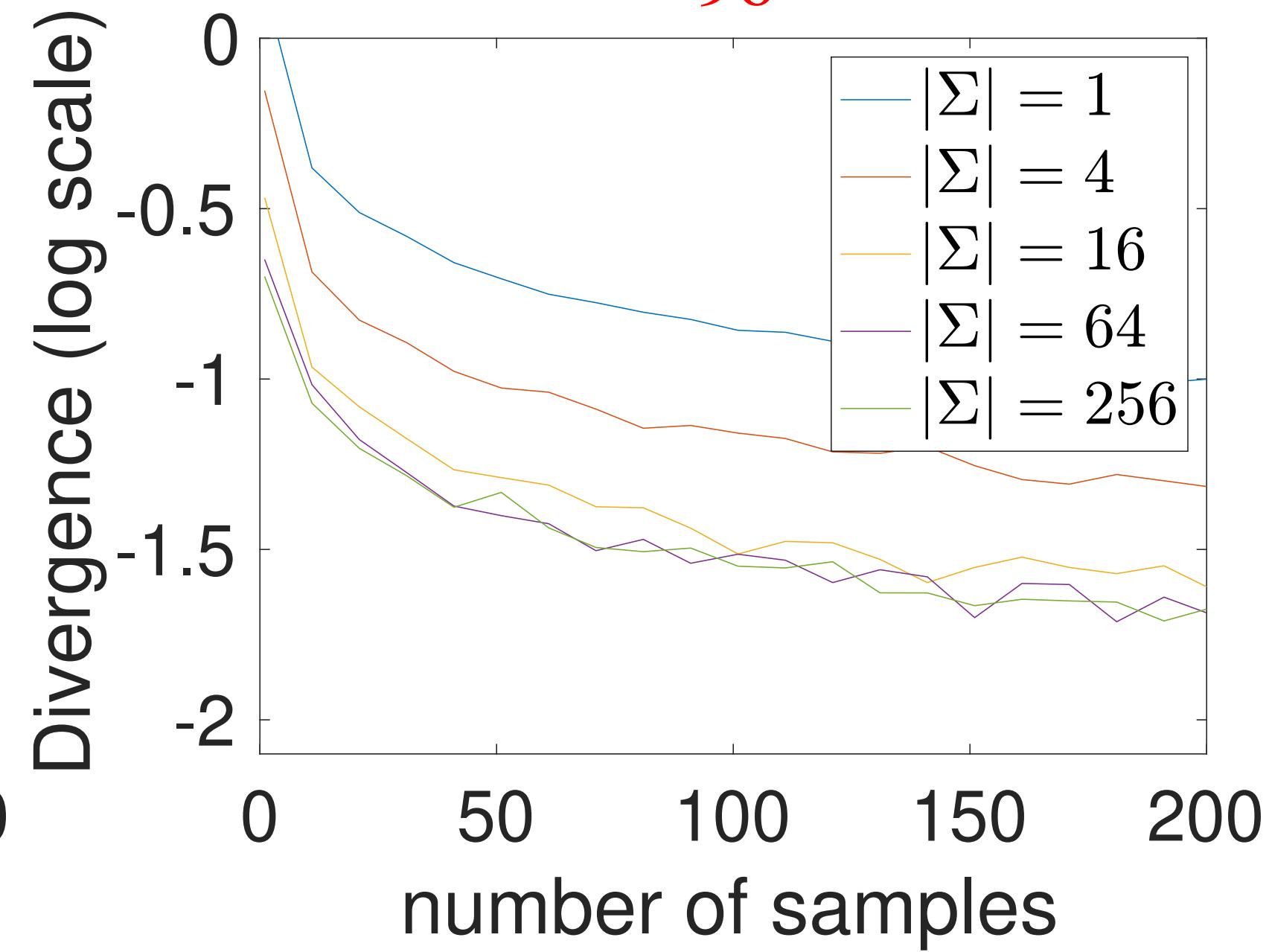
Maximum Mean Discrepancy (MMD)

$$\left| \text{MMD}(Q, P) - \text{MMD}^{\Sigma}(Q_n, P_m) \right| = O \left(C_{\Sigma, k} \left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}} \right) \right), \quad C_{\Sigma, k} = \sqrt{a_{\Sigma, k} + \frac{1 - a_{\Sigma, k}}{|\Sigma|}}$$

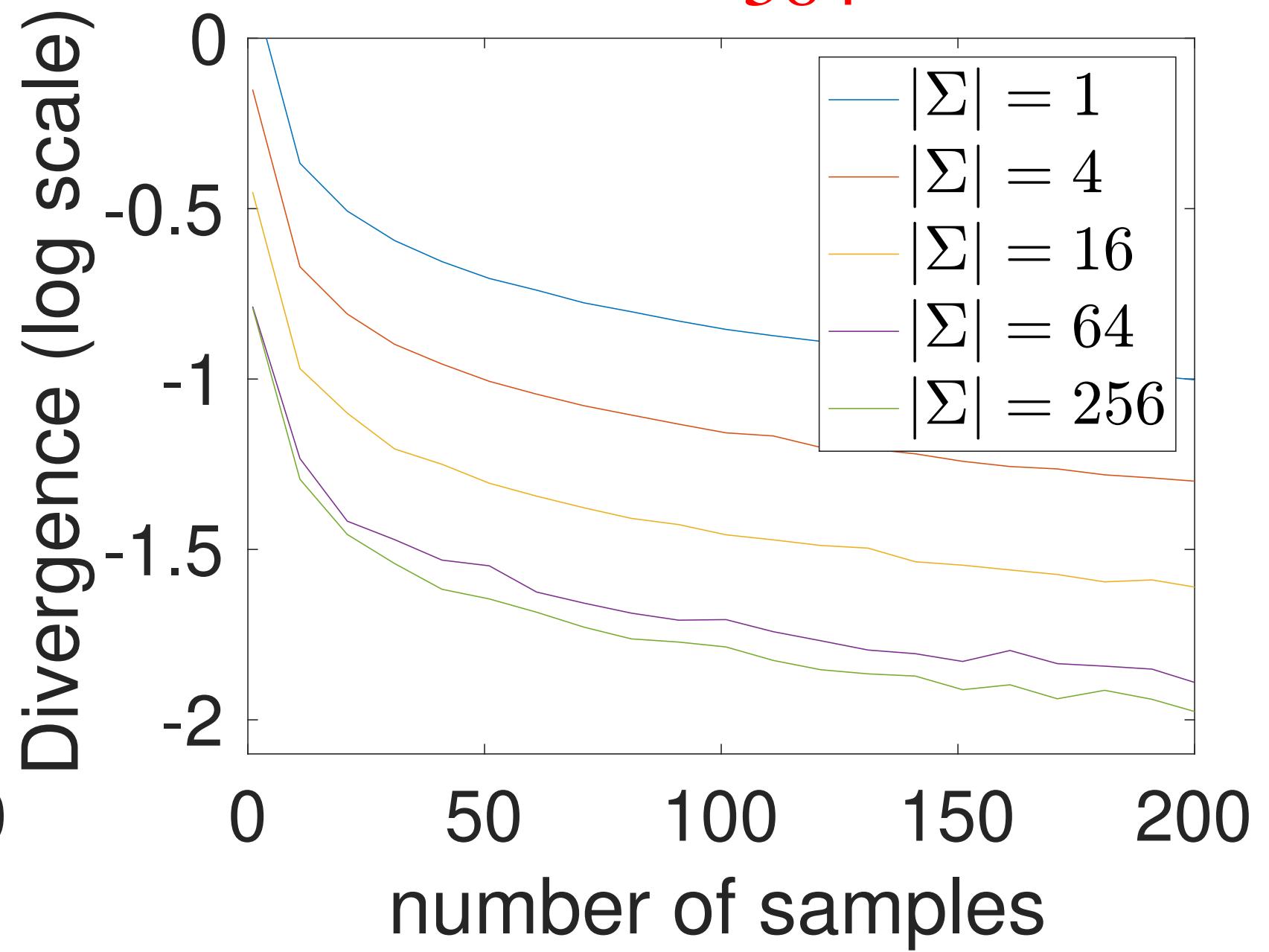
$$s = \frac{2\pi}{24}$$



$$s = \frac{2\pi}{96}$$

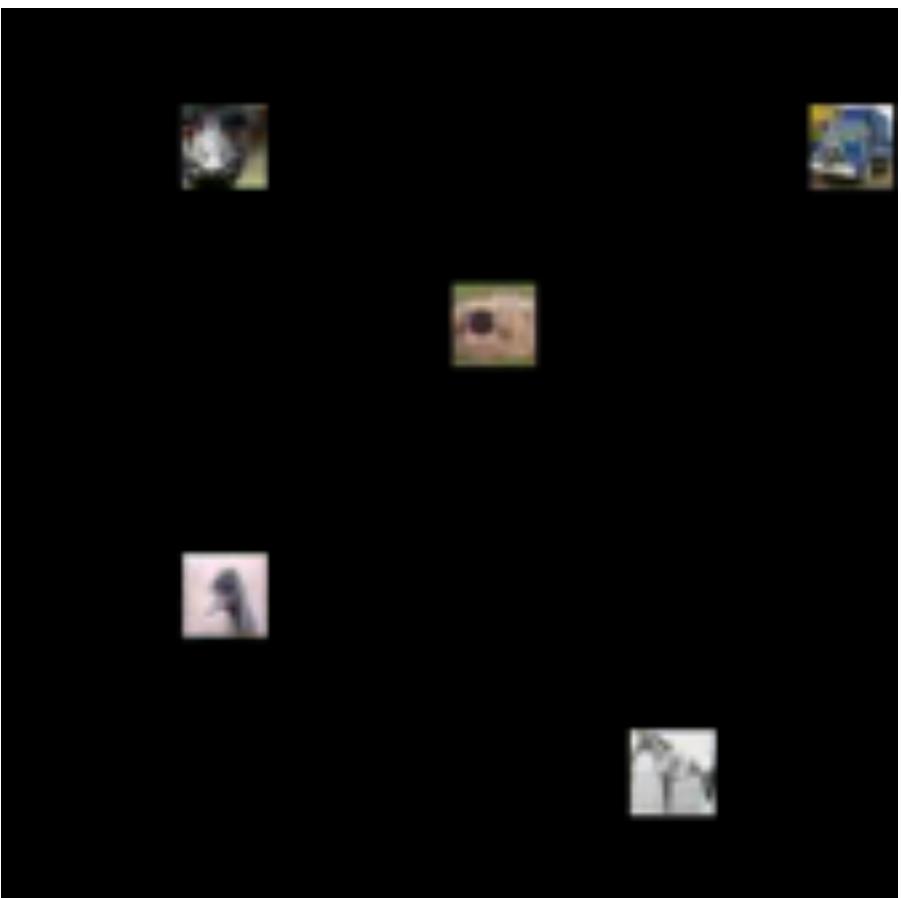
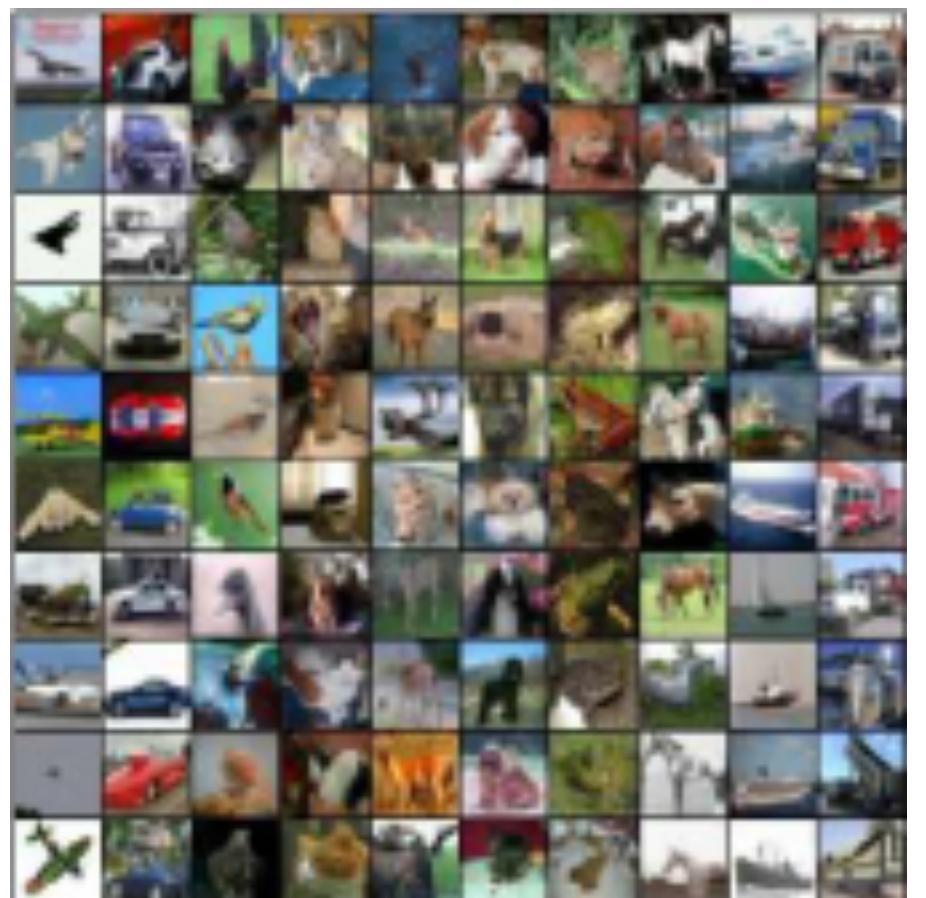


$$s = \frac{2\pi}{384}$$



Missing pieces

- Exact quantification of the improvement
 - Sample complexity and error bound.
- Does it converge? To what solution?
 - Training dynamics of equivariant models

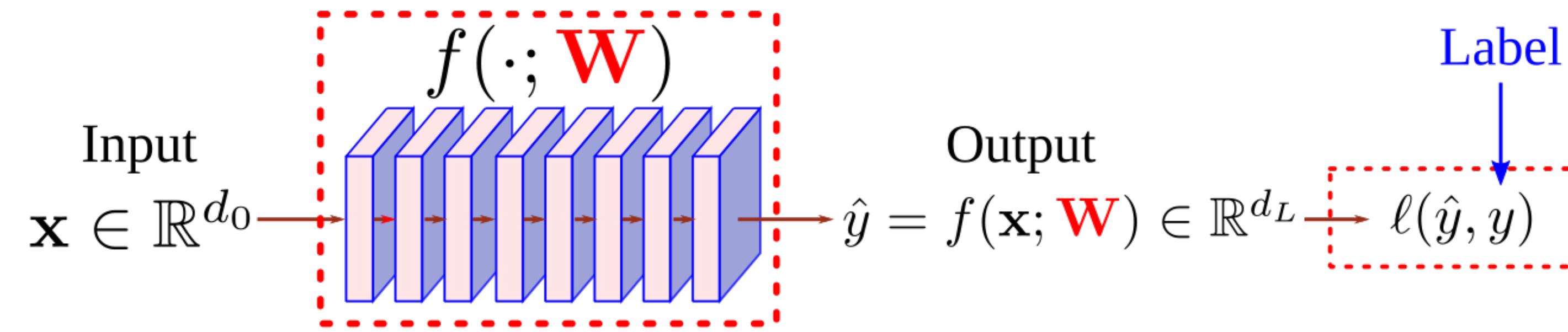


$$\mathbf{W}^* = \arg \min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

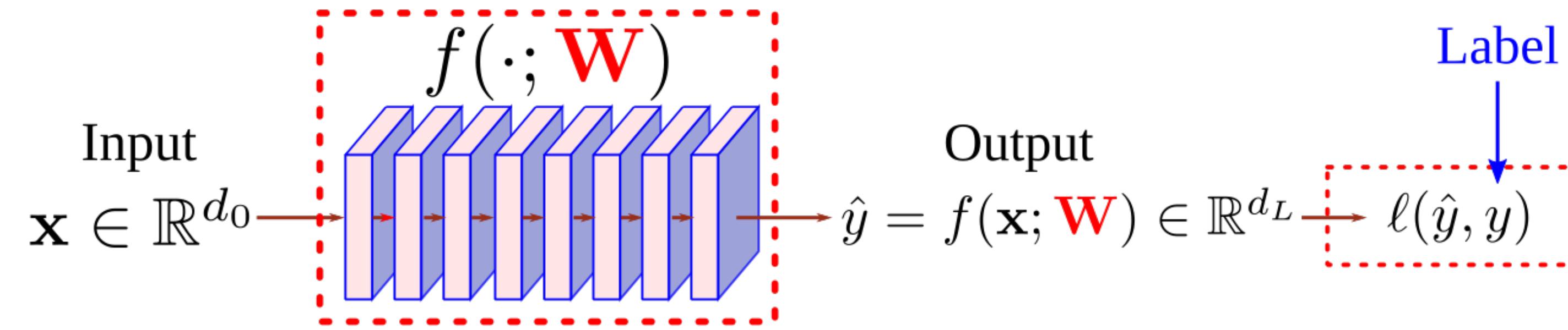
Implicit bias of linear equivariant networks

- Z. Chen and **W. Zhu**. “On the implicit bias of linear equivariant steerable networks”. *NeurIPS* (2023)
- Inspired by [Lawrence et al., *ICML* 2022]

Optimization (training) of G-CNN



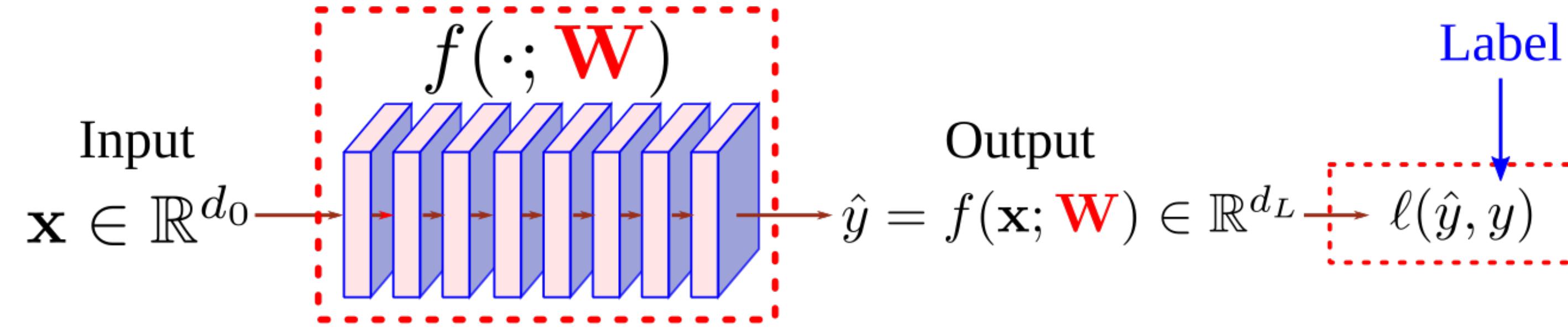
Optimization (training) of G-CNN



- Training a DNN on the a (labeled) data set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$:

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = -\frac{1}{n} \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

Optimization (training) of G-CNN

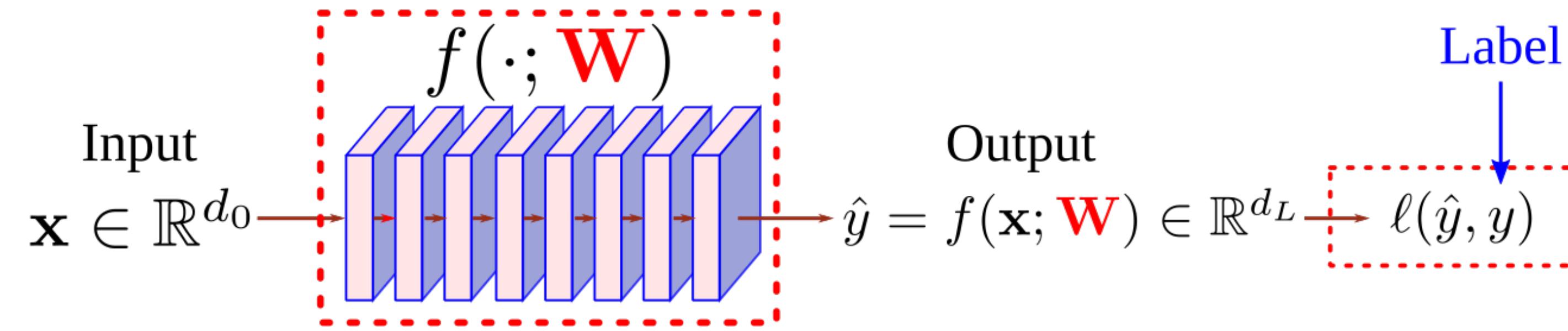


- Training a DNN on the a (labeled) data set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$:

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = -\frac{1}{n} \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

- Design $f(\cdot; \mathbf{W})$ to respect group symmetry—**explicit regularization**.

Optimization (training) of G-CNN



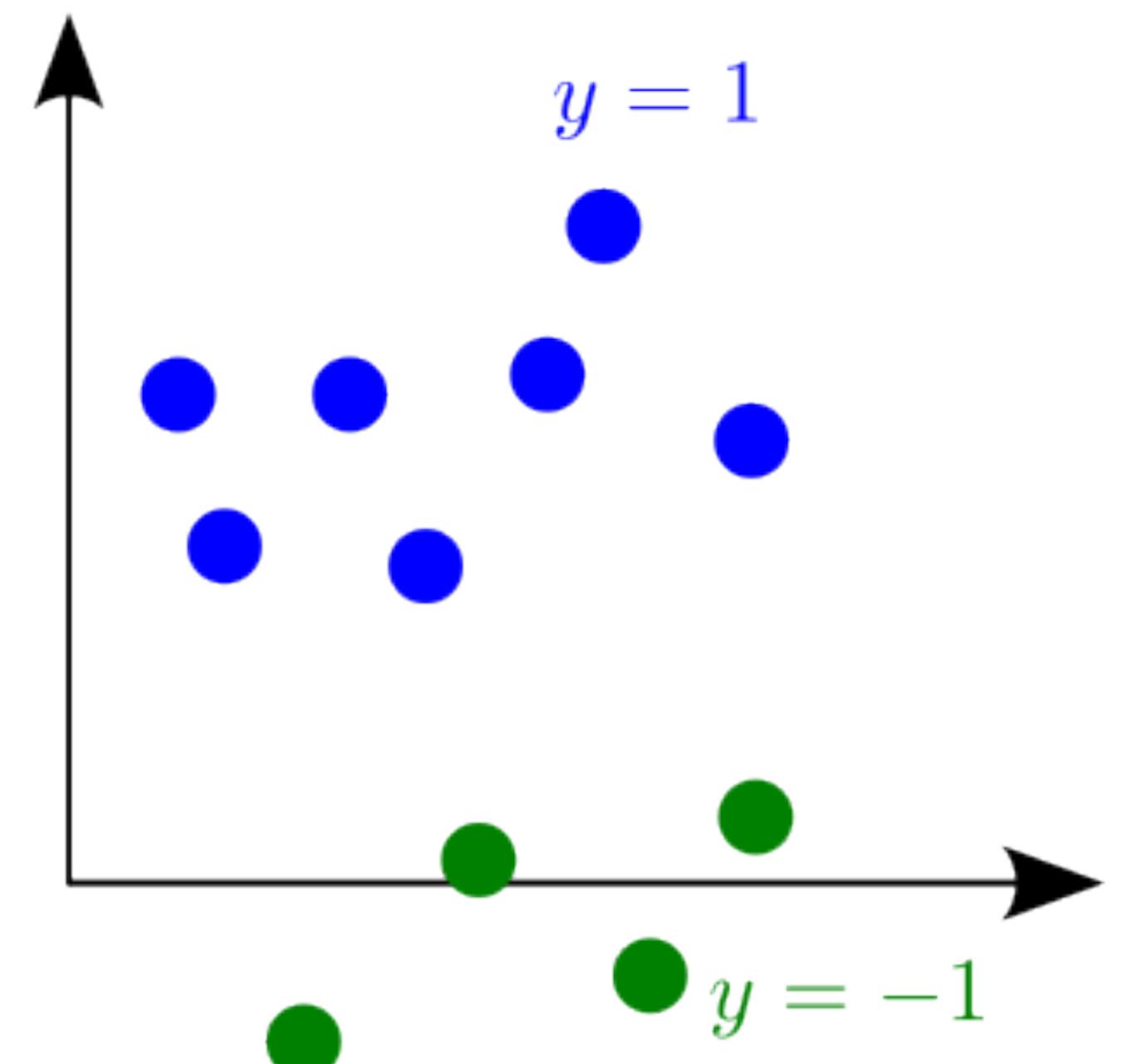
- Training a DNN on the a (labeled) data set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$:

$$\min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = \frac{1}{n} \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

- Design $f(\cdot; \mathbf{W})$ to respect group symmetry—**explicit regularization**.
- **Question:** when trained with gradient-based methods,
 - which solution does it converge to?
 - is it really better than non-equivariant models?

Implicit regularization of training algorithms

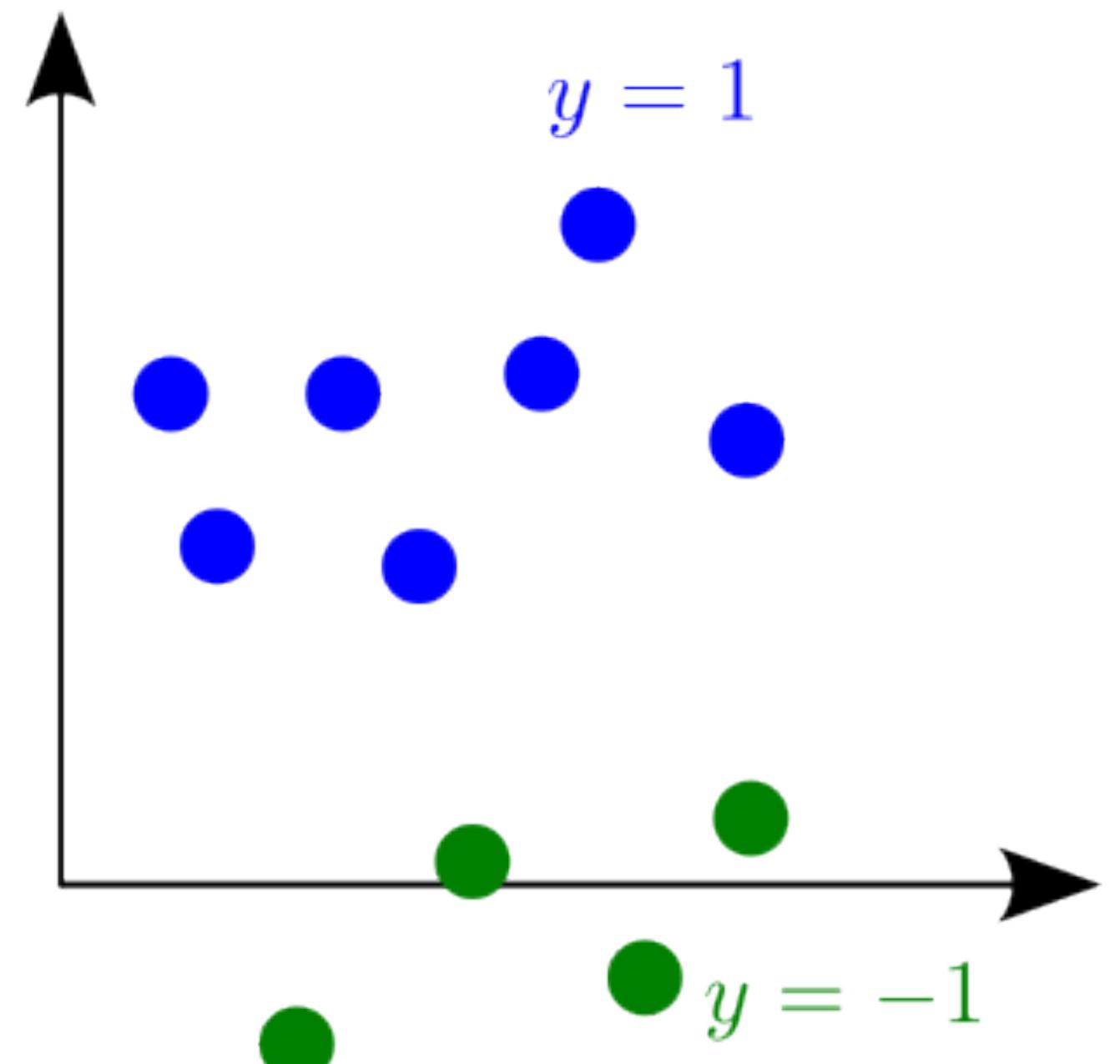
Linear binary classification



Implicit regularization of training algorithms

- $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$, $\mathbf{x}_i \in \mathbb{R}^{d_0}$ and $y_i \in \{\pm 1\}$.

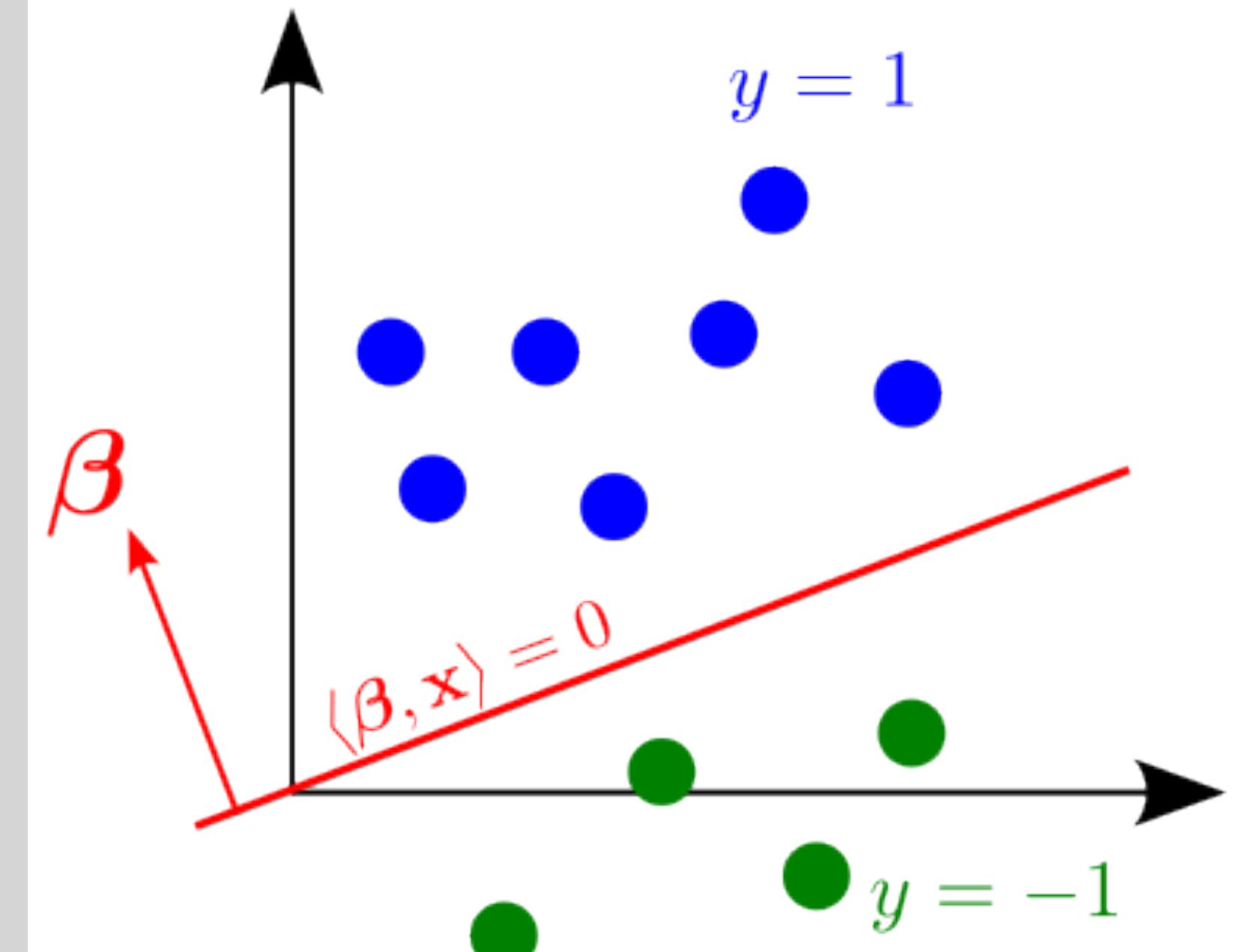
Linear binary classification



Implicit regularization of training algorithms

- $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$, $\mathbf{x}_i \in \mathbb{R}^{d_0}$ and $y_i \in \{\pm 1\}$.
- **Linearly separable:** $\exists \beta^* \in \mathbb{R}^{d_0}$, s.t $y_i \langle \mathbf{x}_i, \beta^* \rangle \geq 1, \forall i \in [n]$.

Linear binary classification



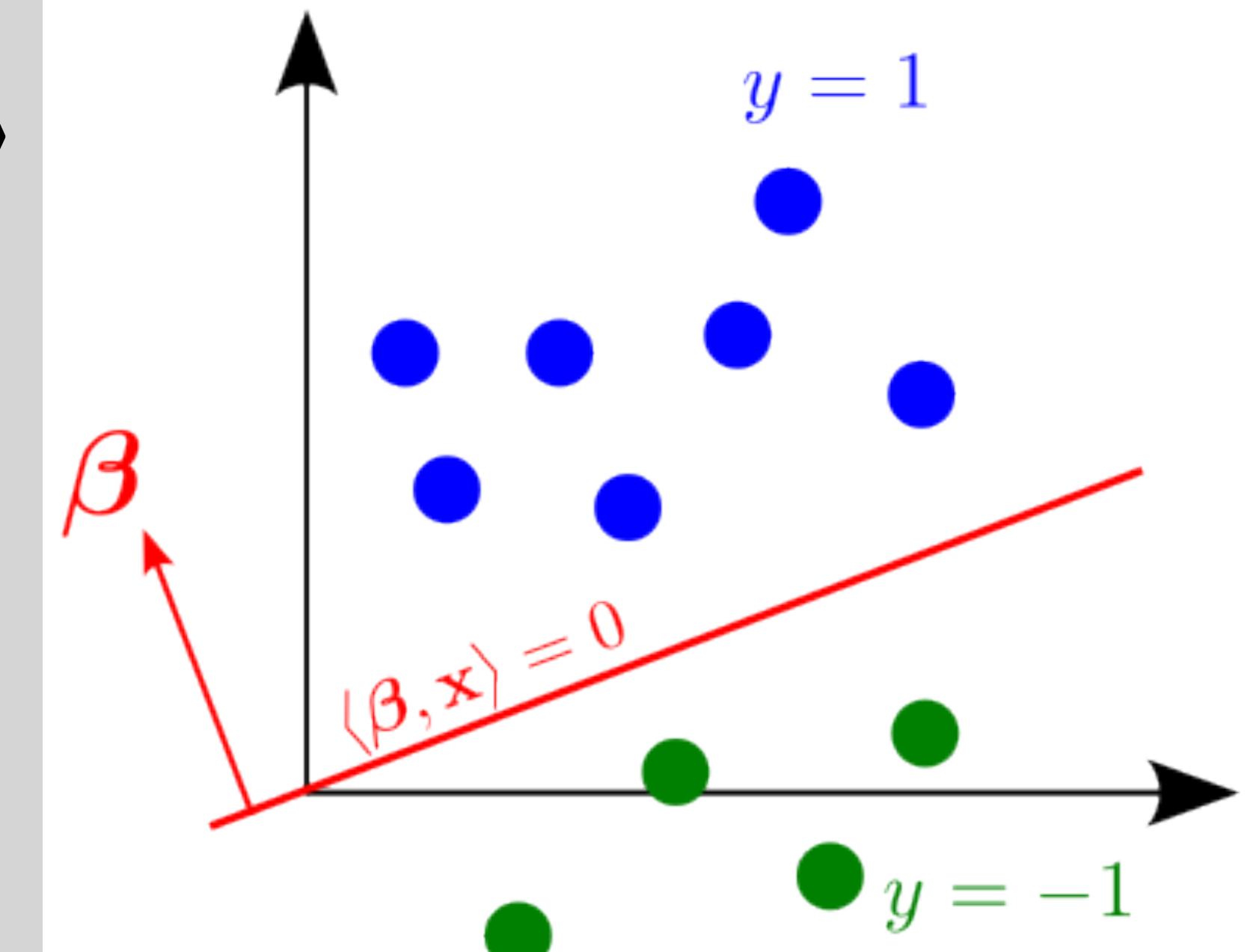
Implicit regularization of training algorithms

- $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$, $\mathbf{x}_i \in \mathbb{R}^{d_0}$ and $y_i \in \{\pm 1\}$.
- **Linearly separable:** $\exists \beta^* \in \mathbb{R}^{d_0}$, s.t $y_i \langle \mathbf{x}_i, \beta^* \rangle \geq 1, \forall i \in [n]$.
- Use **linear fully-connected (fc)** network to parameterize $\langle \mathbf{x}, \beta^* \rangle$

$$f_{\text{fc}}(\mathbf{x}; \mathbf{W}) = \mathbf{w}_L^\top \mathbf{w}_{L-1}^\top \cdots \mathbf{w}_1^\top \mathbf{x} = \langle \mathbf{x}, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle \stackrel{?}{\approx} \langle \mathbf{x}, \beta^* \rangle$$

$$\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_L], \quad \mathcal{P}_{\text{fc}}(\mathbf{W}) = \mathbf{w}_1 \mathbf{w}_2 \cdots \mathbf{w}_L$$

Linear binary classification



Implicit regularization of training algorithms

- $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$, $\mathbf{x}_i \in \mathbb{R}^{d_0}$ and $y_i \in \{\pm 1\}$.
- **Linearly separable:** $\exists \beta^* \in \mathbb{R}^{d_0}$, s.t $y_i \langle \mathbf{x}_i, \beta^* \rangle \geq 1, \forall i \in [n]$.
- Use **linear fully-connected (fc)** network to parameterize $\langle \mathbf{x}, \beta^* \rangle$

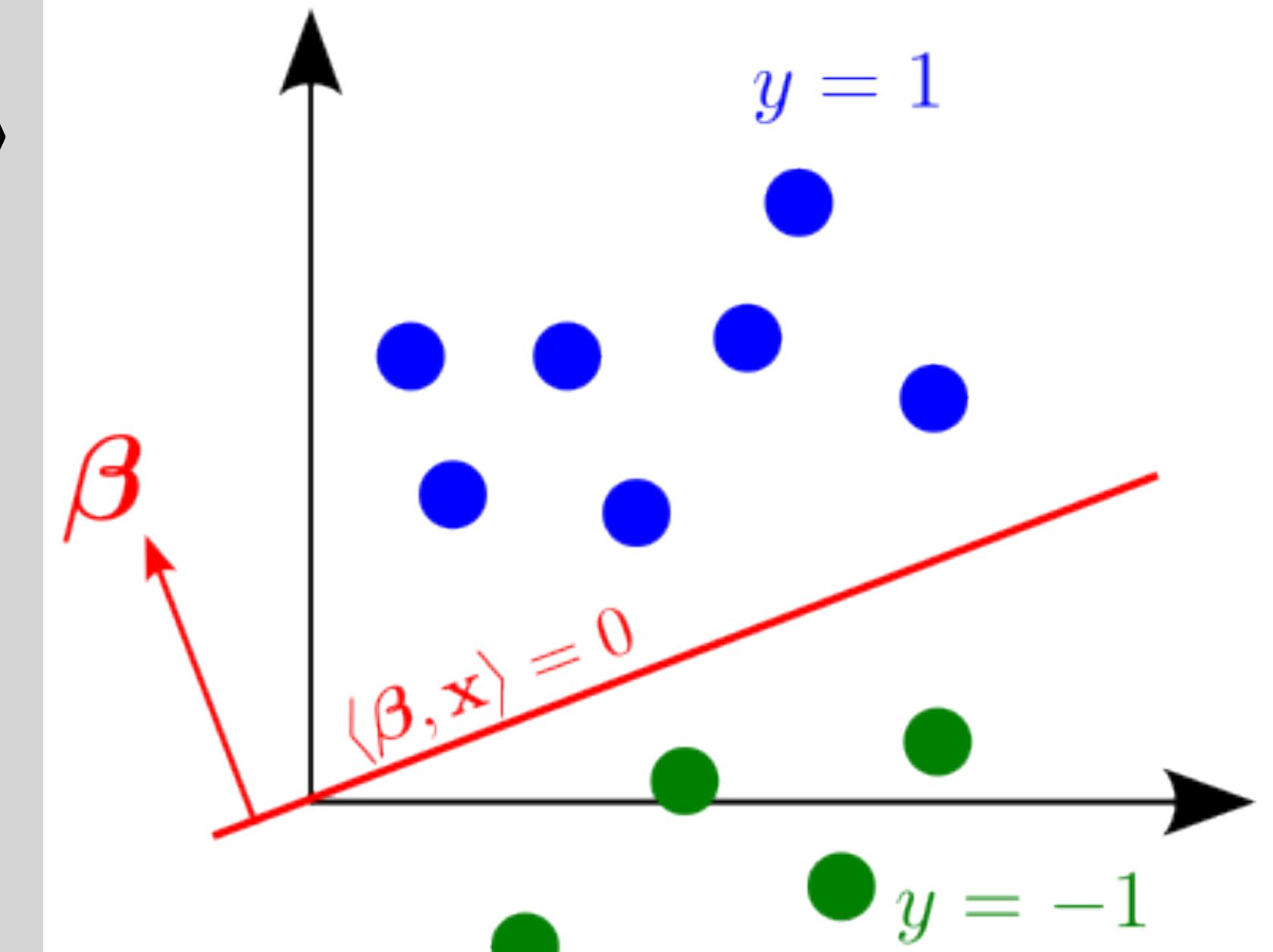
$$f_{\text{fc}}(\mathbf{x}; \mathbf{W}) = \mathbf{w}_L^\top \mathbf{w}_{L-1}^\top \cdots \mathbf{w}_1^\top \mathbf{x} = \langle \mathbf{x}, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle \stackrel{?}{\approx} \langle \mathbf{x}, \beta^* \rangle$$

$$\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_L], \quad \mathcal{P}_{\text{fc}}(\mathbf{W}) = \mathbf{w}_1 \mathbf{w}_2 \cdots \mathbf{w}_L$$

- Regression based on $\ell_{\text{exp}}(\hat{y}, y) = \exp(-\hat{y}y)$

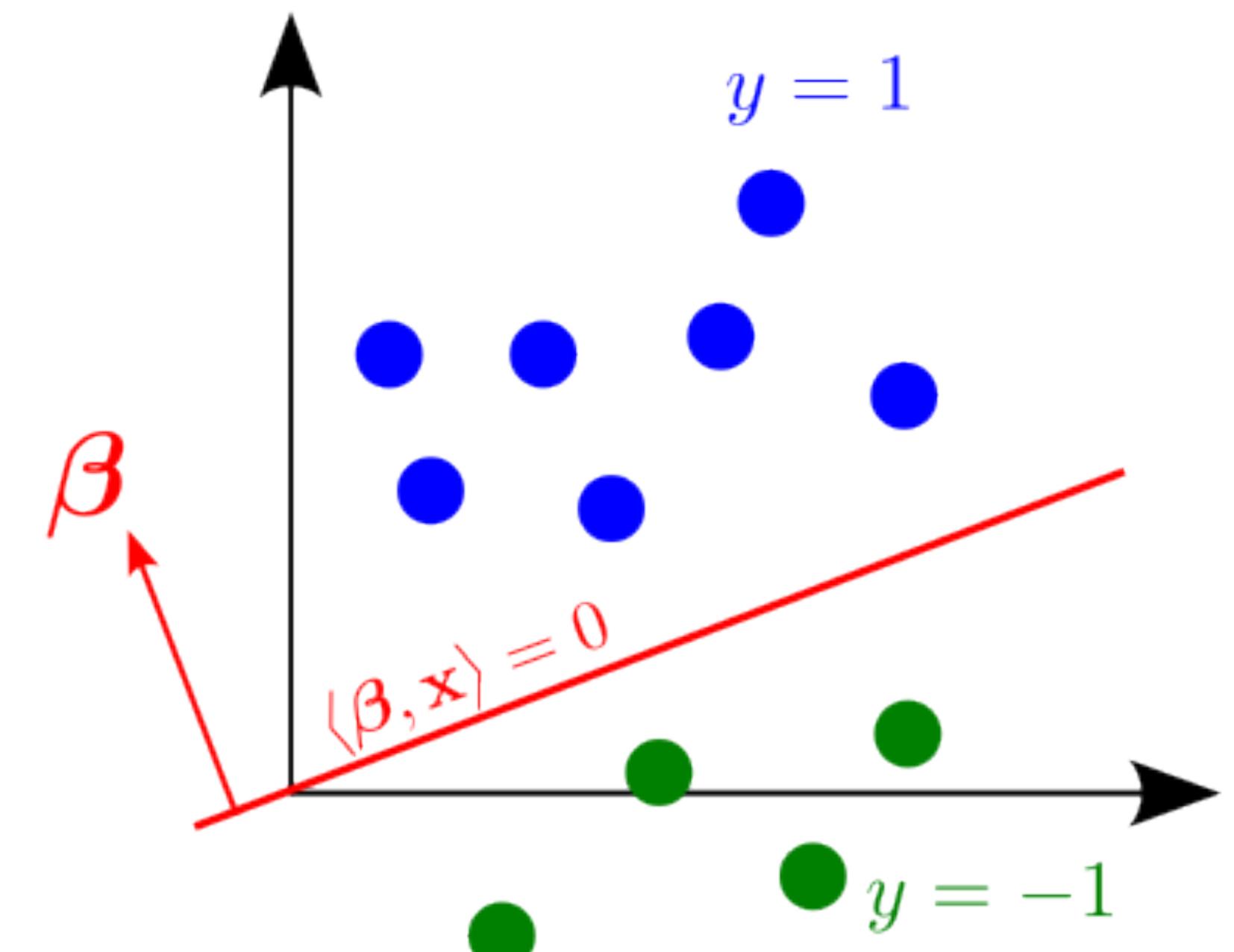
$$\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\text{exp}} \left(\langle \mathbf{x}_i, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle, y_i \right)$$

Linear binary classification



Implicit regularization of training algorithms

Linear binary classification



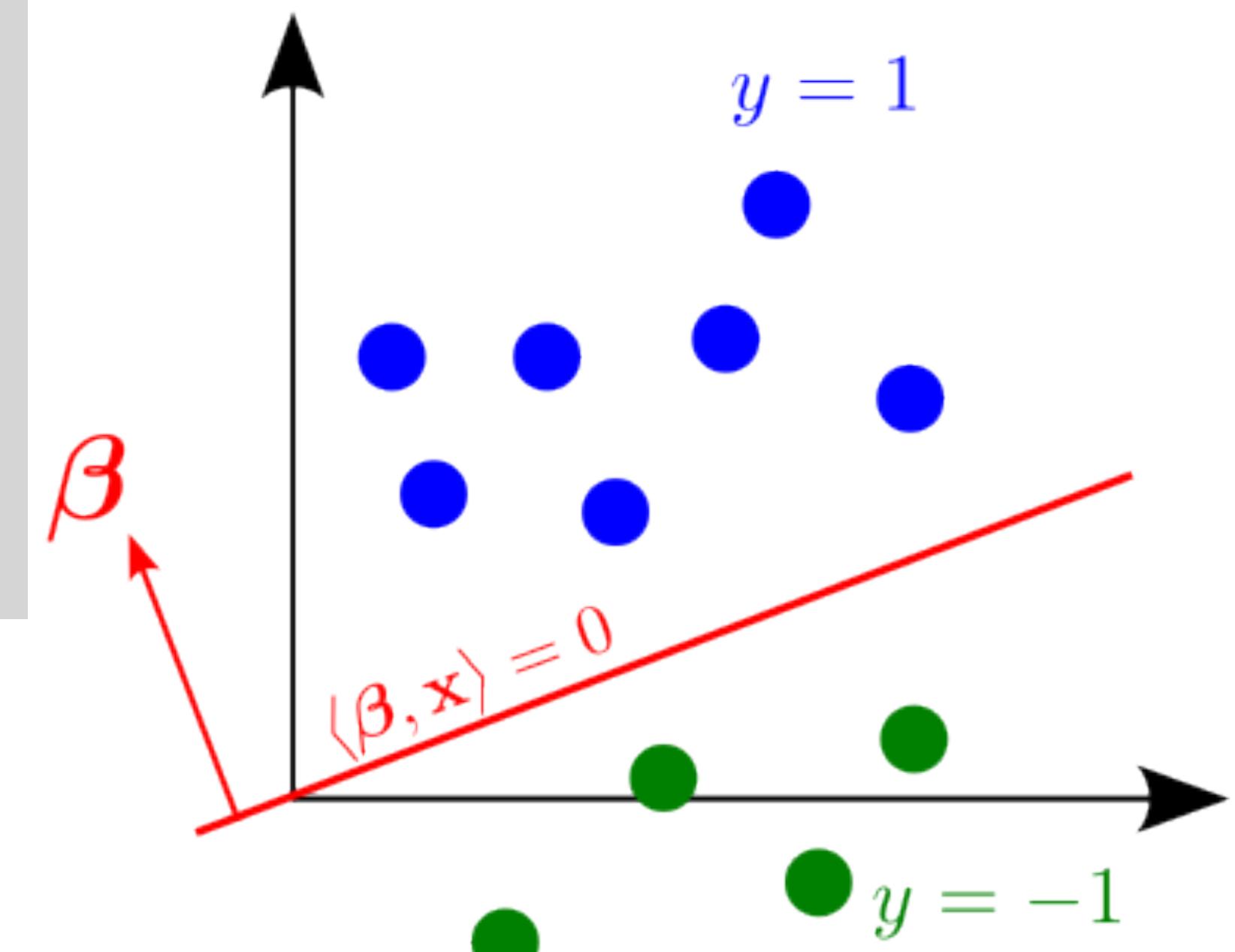
Implicit regularization of training algorithms

$$\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\exp} \left(\langle \mathbf{x}_i, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle, y_i \right)$$

- Trained under **gradient flow (GF)**:

$$\frac{d\mathbf{W}}{dt} = - \nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S)$$

Linear binary classification



Implicit regularization of training algorithms

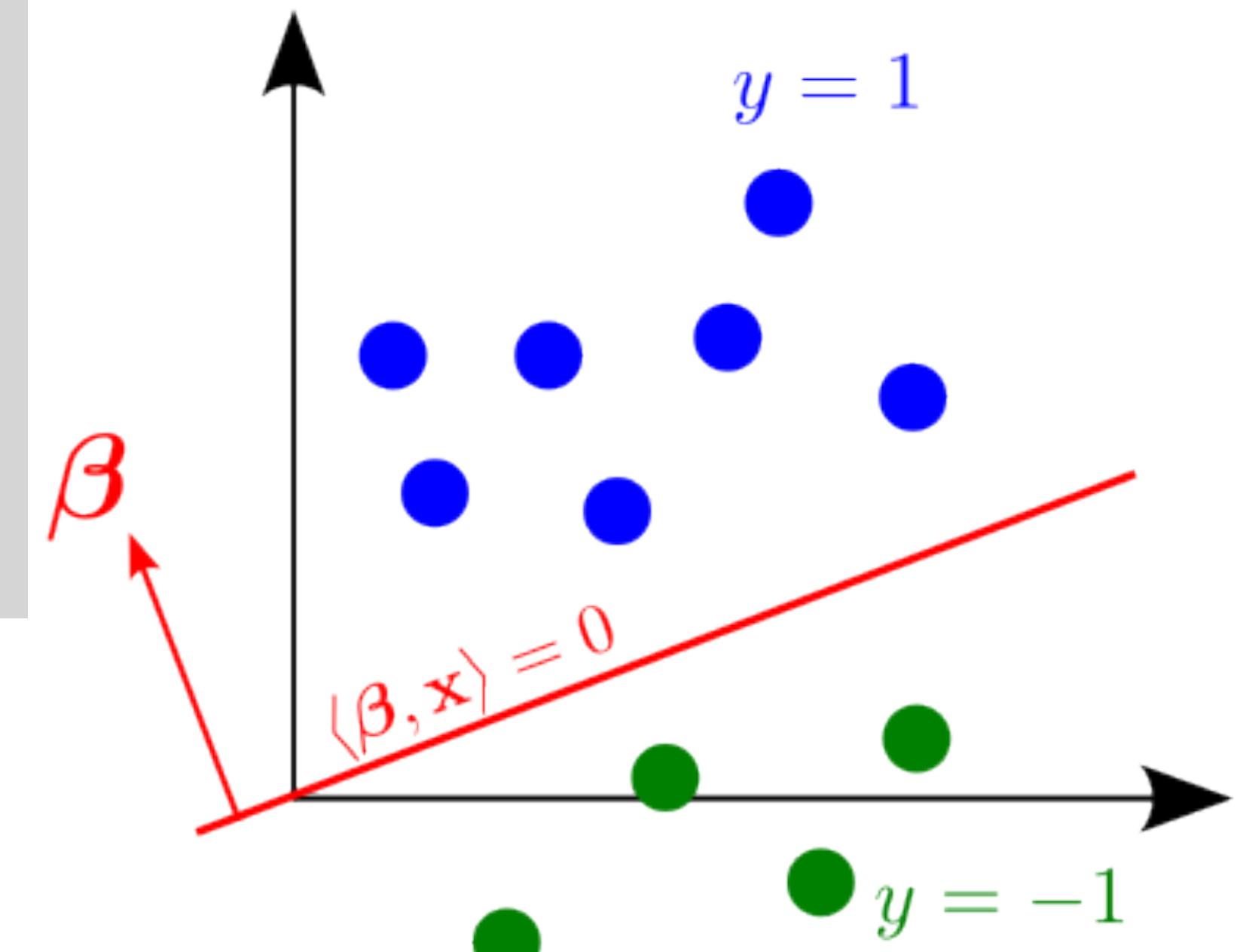
$$\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\exp} \left(\langle \mathbf{x}_i, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle, y_i \right)$$

- Trained under **gradient flow (GF)**:

$$\frac{d\mathbf{W}}{dt} = - \nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S)$$

Question: to what does $\beta_{\text{fc}}(t) = \mathcal{P}_{\text{fc}}(\mathbf{W}(t))$ converge?

Linear binary classification



Implicit regularization of training algorithms

$$\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\exp} \left(\langle \mathbf{x}_i, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle, y_i \right)$$

- Trained under **gradient flow (GF)**:

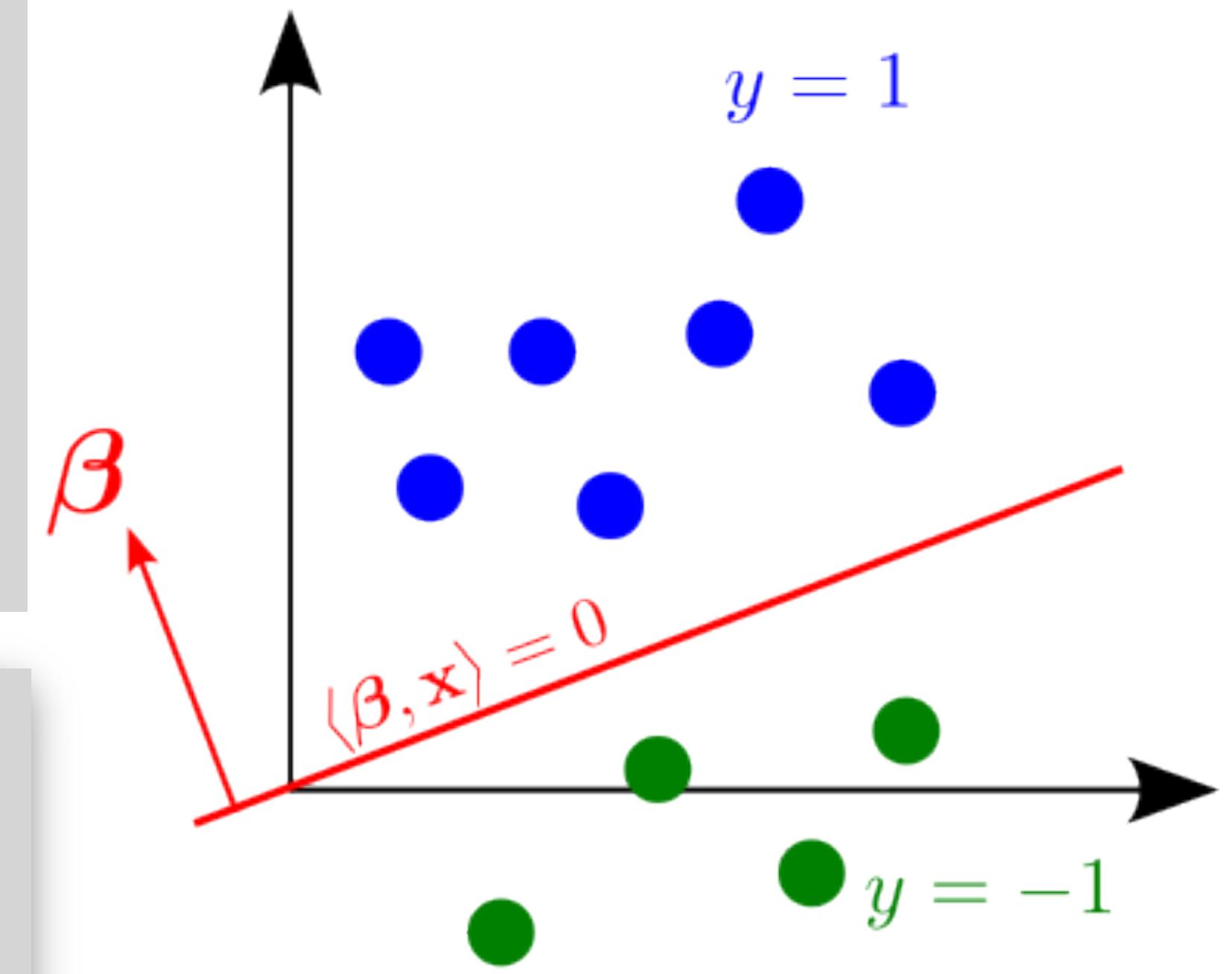
$$\frac{d\mathbf{W}}{dt} = - \nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S)$$

Question: to what does $\beta_{\text{fc}}(t) = \mathcal{P}_{\text{fc}}(\mathbf{W}(t))$ converge?

Fact [Ji and Telgarsky, *ICLR* 2018], [Yun et al., *ICLR* 2021]

- $\beta_{\text{fc}}^\infty = \lim_{t \rightarrow \infty} \beta_{\text{fc}}(t)/\|\beta_{\text{fc}}(t)\|$ exists.

Linear binary classification



Implicit regularization of training algorithms

$$\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\exp} \left(\langle \mathbf{x}_i, \mathcal{P}_{\text{fc}}(\mathbf{W}) \rangle, y_i \right)$$

- Trained under **gradient flow (GF)**:

$$\frac{d\mathbf{W}}{dt} = - \nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{fc}}}(\mathbf{W}; S)$$

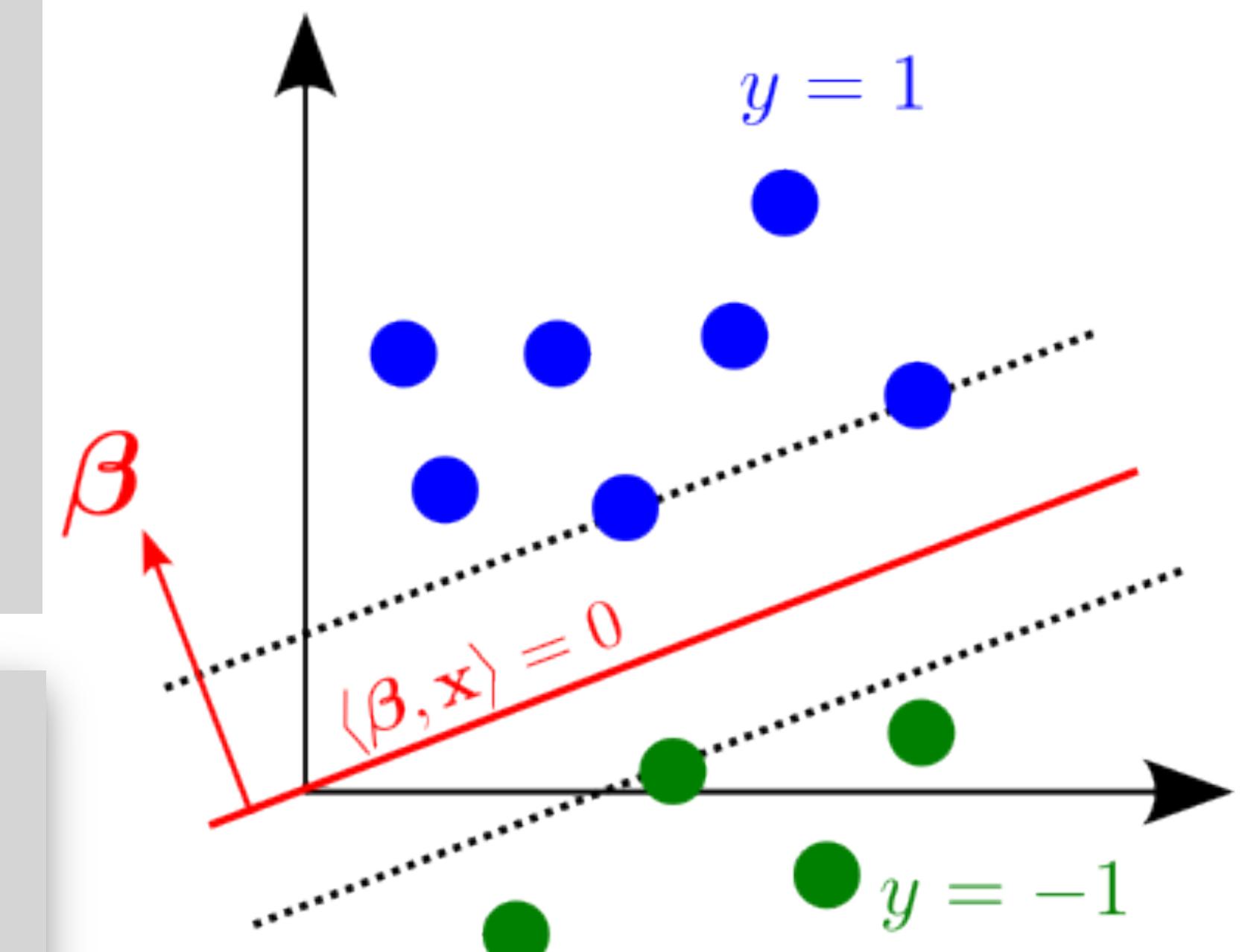
Question: to what does $\beta_{\text{fc}}(t) = \mathcal{P}_{\text{fc}}(\mathbf{W}(t))$ converge?

Fact [Ji and Telgarsky, *ICLR* 2018], [Yun et al., *ICLR* 2021]

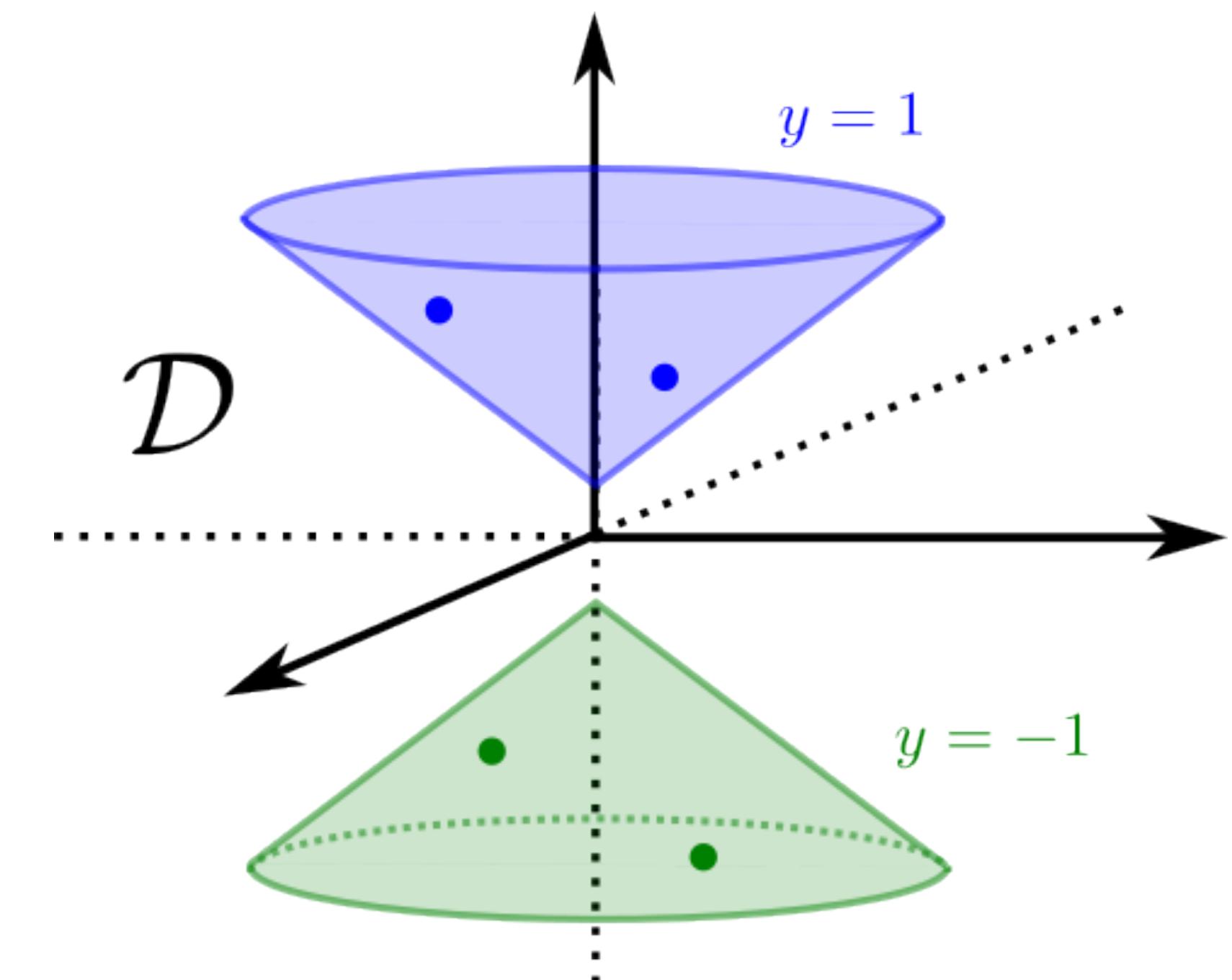
- $\beta_{\text{fc}}^\infty = \lim_{t \rightarrow \infty} \beta_{\text{fc}}(t)/\|\beta_{\text{fc}}(t)\|$ exists.

- β_{fc}^∞ is the the **max- L^2 -margin** support vector machine (SVM).

Linear binary classification

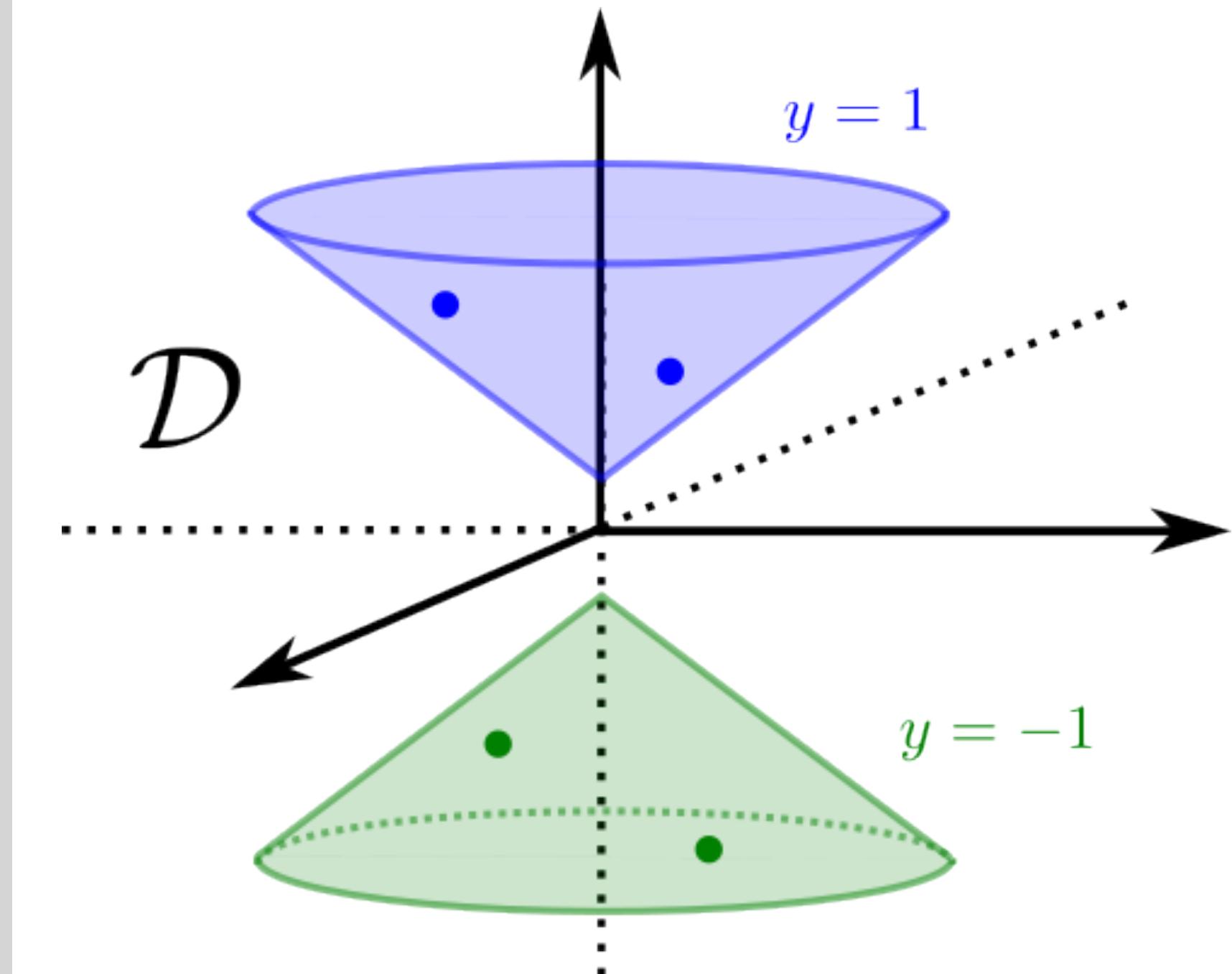


Group-invariant binary classification



Group-invariant binary classification

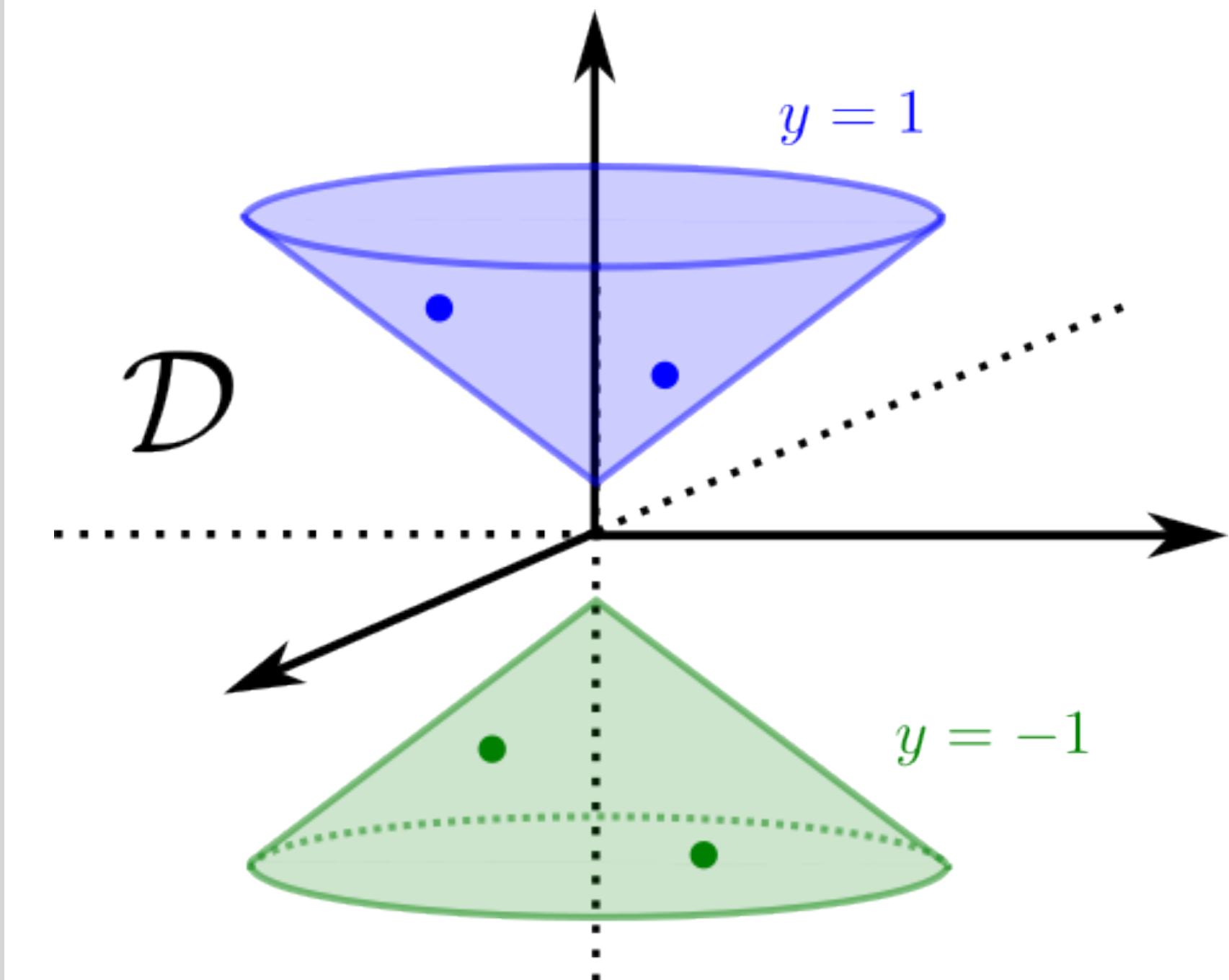
- Assume $S \sim \mathcal{D}$, and \mathcal{D} is invariant to a linear G -action.



Group-invariant binary classification

- Assume $S \sim \mathcal{D}$, and \mathcal{D} is invariant to a linear G -action.
- Parameterize the invariant linear predictor β using a **G-CNN**,

$$f_{\text{inv}}(\mathbf{x}; \mathbf{W}) = \langle \mathbf{x}, \mathcal{P}_{\text{inv}}(\mathbf{W}) \rangle$$



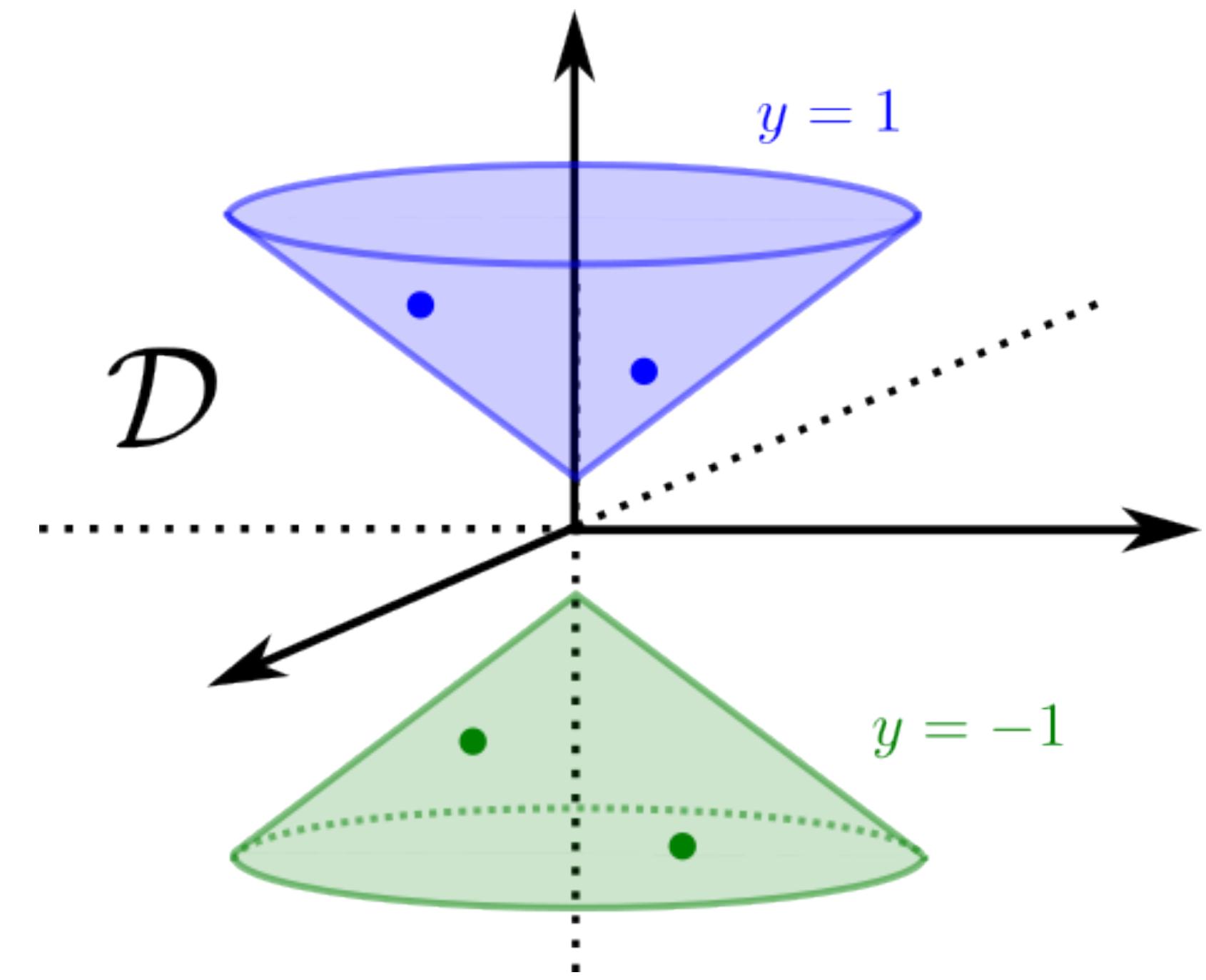
Group-invariant binary classification

- Assume $S \sim \mathcal{D}$, and \mathcal{D} is invariant to a linear G -action.
- Parameterize the invariant linear predictor β using a **G-CNN**,

$$f_{\text{inv}}(\mathbf{x}; \mathbf{W}) = \langle \mathbf{x}, \mathcal{P}_{\text{inv}}(\mathbf{W}) \rangle$$

- Regression: $\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{inv}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\text{exp}}\left(\langle \mathbf{x}_i, \mathcal{P}_{\text{inv}}(\mathbf{W}) \rangle, y_i\right)$

- Gradient flow: $\frac{d\mathbf{W}}{dt} = -\nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{inv}}}(\mathbf{W}; S)$



Group-invariant binary classification

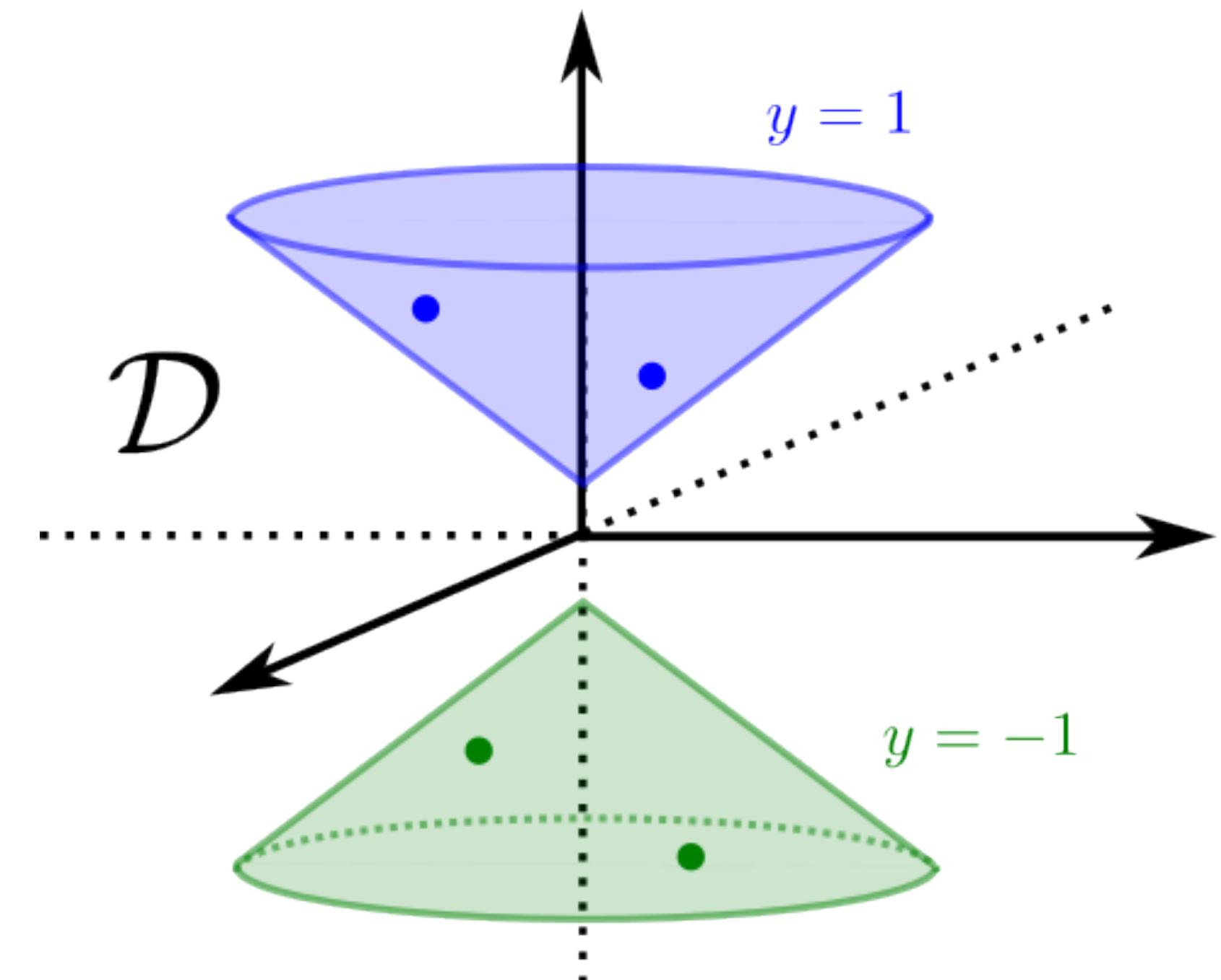
- Assume $S \sim \mathcal{D}$, and \mathcal{D} is invariant to a linear G -action.
- Parameterize the invariant linear predictor β using a **G-CNN**,

$$f_{\text{inv}}(\mathbf{x}; \mathbf{W}) = \langle \mathbf{x}, \mathcal{P}_{\text{inv}}(\mathbf{W}) \rangle$$

- Regression: $\min_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{inv}}}(\mathbf{W}; S) = \sum_{i=1}^n \ell_{\text{exp}}\left(\langle \mathbf{x}_i, \mathcal{P}_{\text{inv}}(\mathbf{W}) \rangle, y_i\right)$

- Gradient flow: $\frac{d\mathbf{W}}{dt} = -\nabla_{\mathbf{W}} \mathcal{L}_{\mathcal{P}_{\text{inv}}}(\mathbf{W}; S)$

Question: to what does $\beta_{\text{inv}}(t) = \mathcal{P}_{\text{inv}}(\mathbf{W}(t))$ converge?



Group-invariant binary classification

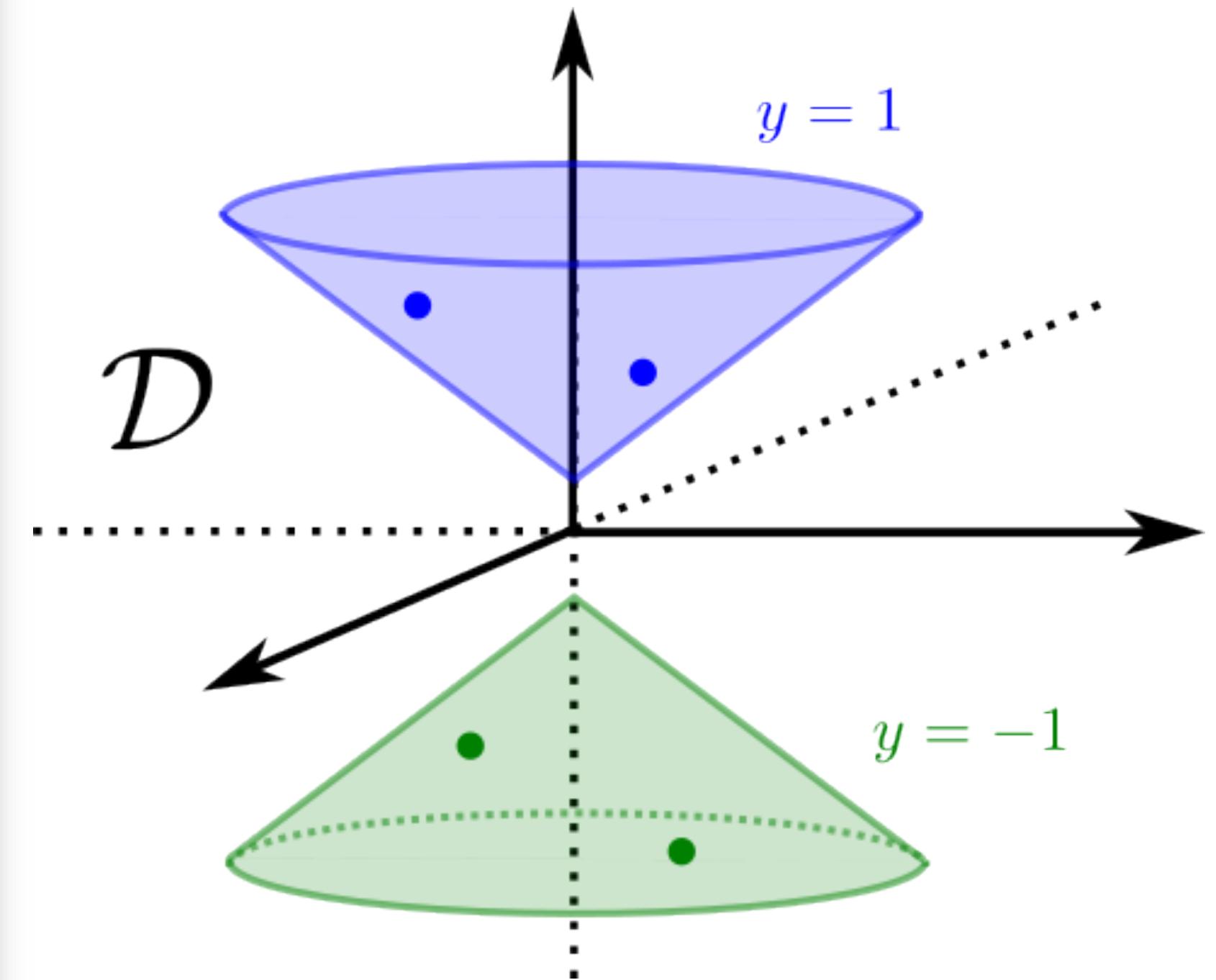
Group-invariant binary classification

Question: to what does $\beta_{\text{inv}}(t) = \mathcal{P}_{\text{inv}}(\mathbf{W}(t))$ converge?

Theorem [Chen and Z., NeurIPS 2023]

If the input linear G -action is unitary, then

- $\beta_{\text{inv}}^\infty = \lim_{t \rightarrow \infty} \beta_{\text{inv}}(t)/\|\beta_{\text{inv}}(t)\|$ exists.



Group-invariant binary classification

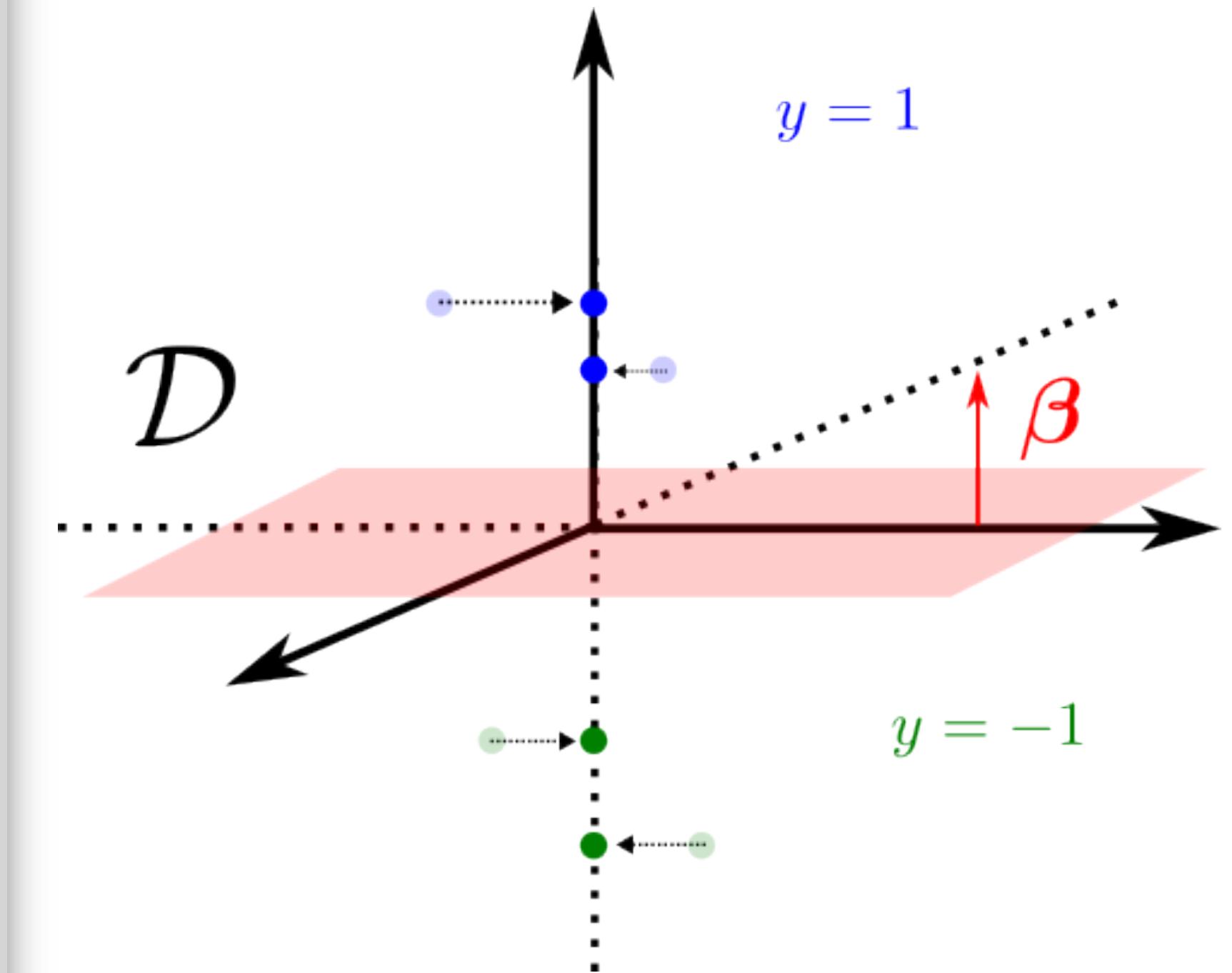
Question: to what does $\beta_{\text{inv}}(t) = \mathcal{P}_{\text{inv}}(\mathbf{W}(t))$ converge?

Theorem [Chen and Z., NeurIPS 2023]

If the input linear G -action is unitary, then

- $\beta_{\text{inv}}^\infty = \lim_{t \rightarrow \infty} \beta_{\text{inv}}(t)/\|\beta_{\text{inv}}(t)\|$ exists.
- $\beta_{\text{inv}}^\infty$ is the max-margin SVM on the **transformed dataset**

$$\bar{\mathcal{S}} = \{(\bar{\mathbf{x}}_i, y_i) : i \in [n]\}, \text{ where } \bar{\mathbf{x}} = \frac{1}{|G|} \sum_{g \in G} g\mathbf{x}$$



Group-invariant binary classification

Question: to what does $\beta_{\text{inv}}(t) = \mathcal{P}_{\text{inv}}(\mathbf{W}(t))$ converge?

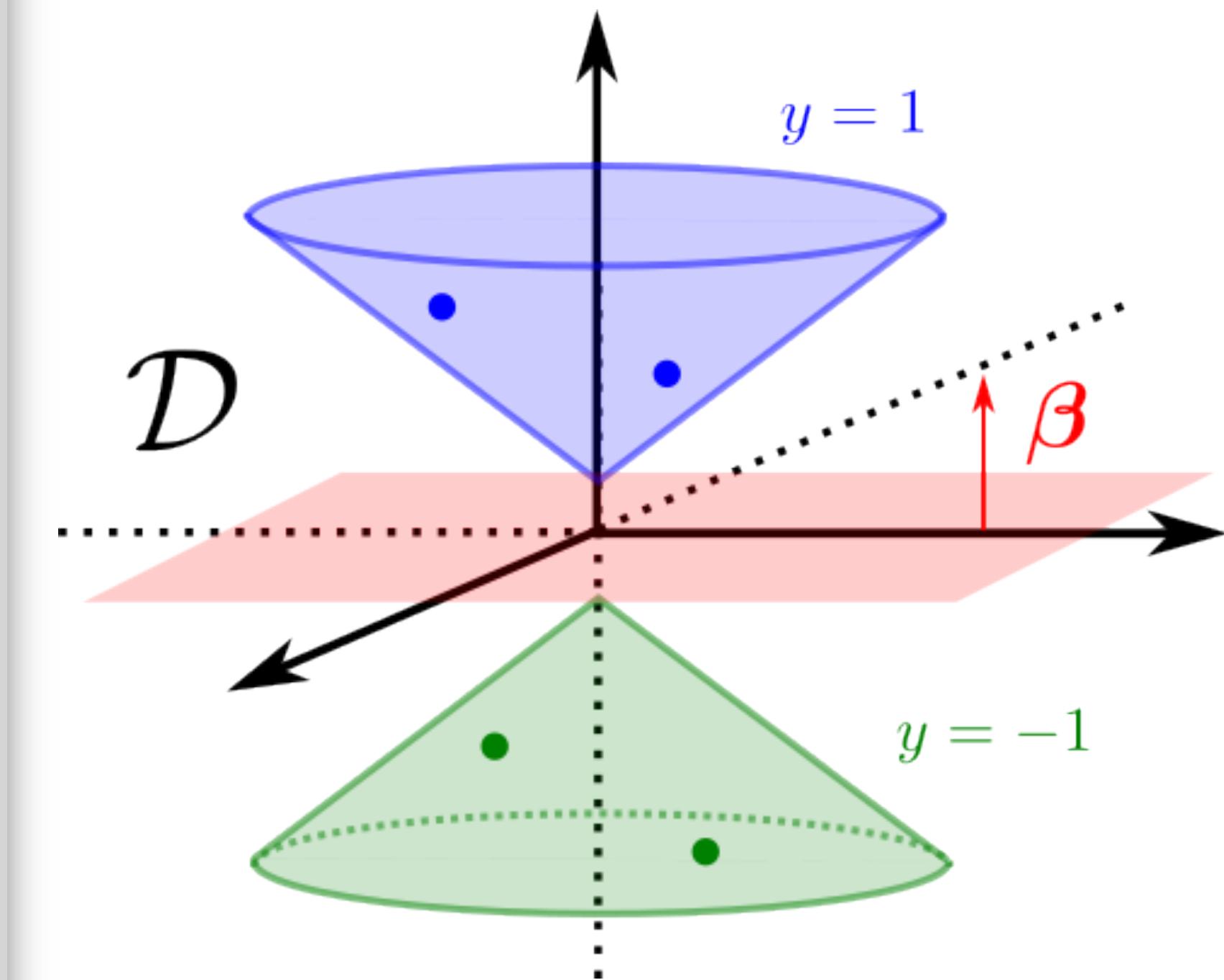
Theorem [Chen and Z., NeurIPS 2023]

If the input linear G -action is unitary, then

- $\beta_{\text{inv}}^\infty = \lim_{t \rightarrow \infty} \beta_{\text{inv}}(t)/\|\beta_{\text{inv}}(t)\|$ exists.
- $\beta_{\text{inv}}^\infty$ is the max-margin SVM on the **transformed dataset**

$$\bar{S} = \{(\bar{\mathbf{x}}_i, y_i) : i \in [n]\}, \text{ where } \bar{\mathbf{x}} = \frac{1}{|G|} \sum_{g \in G} g\mathbf{x}$$

- $\beta_{\text{inv}}^\infty$ is the unique max-margin **invariant** SVM on the **original dataset** $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$



Implications

Implications

Corollary (G-CNN vs data augmentation)

- $\beta_{\text{inv}}^\infty$: linear **G-CNN** trained on $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$.
- β_{fc}^∞ : linear fully-connected network trained on $S_{\text{aug}} = \{(g\mathbf{x}_i, y_i) : i \in [n], g \in G\}$.

$$\beta_{\text{steer}}^\infty = \beta_{\text{fc}}^\infty$$

Implications

Corollary (G-CNN vs data augmentation)

- $\beta_{\text{inv}}^\infty$: linear **G-CNN** trained on $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$.
- β_{fc}^∞ : linear fully-connected network trained on $S_{\text{aug}} = \{(g\mathbf{x}_i, y_i) : i \in [n], g \in G\}$.

$$\beta_{\text{steer}}^\infty = \beta_{\text{fc}}^\infty$$

- Equivariant neural networks is equivalent to data augmentation.

Implications

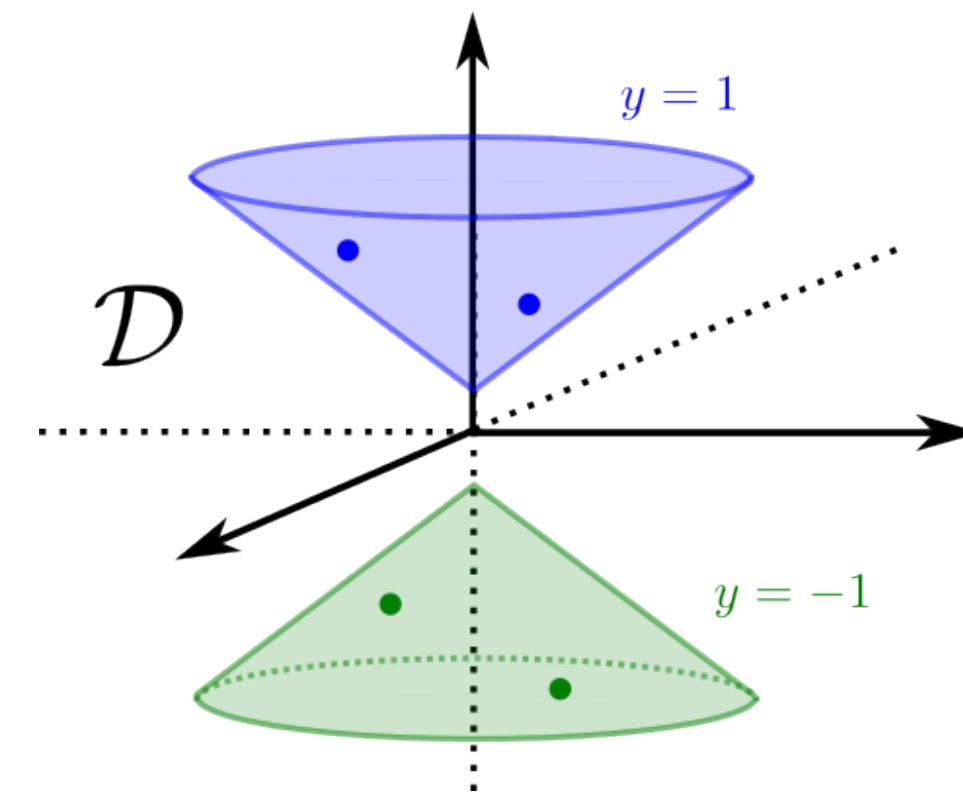
Corollary (G-CNN vs data augmentation)

- $\beta_{\text{inv}}^\infty$: linear **G-CNN** trained on $S = \{(\mathbf{x}_i, y_i) : i \in [n]\}$.
- β_{fc}^∞ : linear fully-connected network trained on $S_{\text{aug}} = \{(g\mathbf{x}_i, y_i) : i \in [n], g \in G\}$.

$$\beta_{\text{steer}}^\infty = \beta_{\text{fc}}^\infty$$

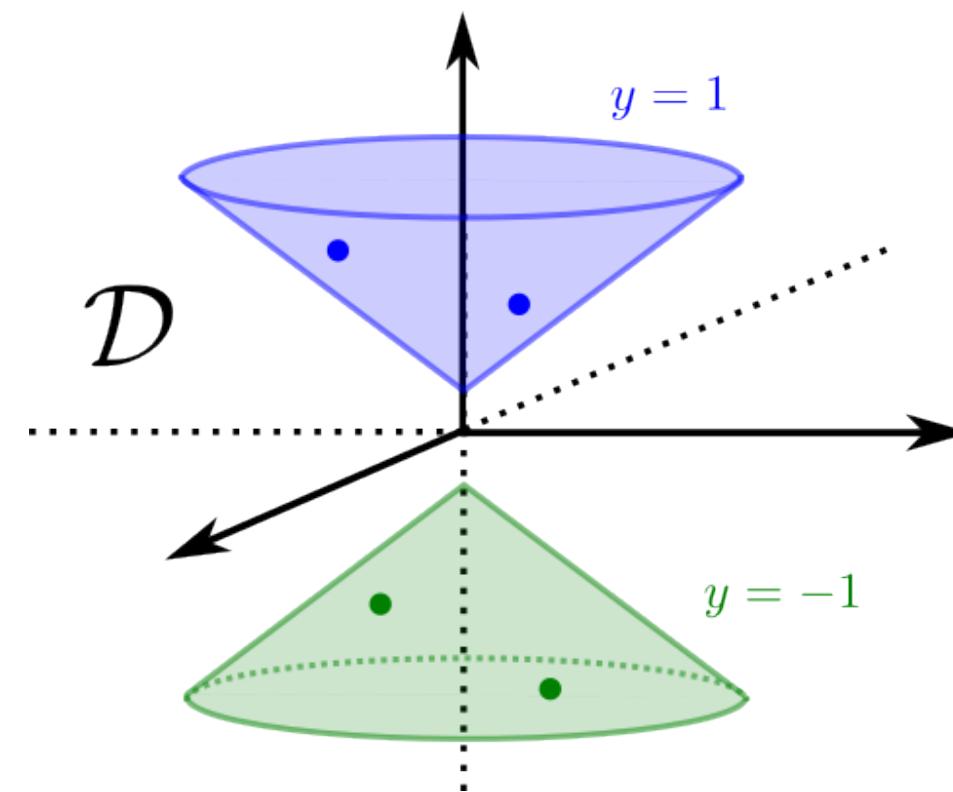
- Equivariant neural networks is equivalent to data augmentation.
- Caveat:
 - Full data augmentation on the entire group G .
 - Unitary input action.
 - Only linear models.

Improved generalization



Improved generalization

- G -invariant distribution \mathcal{D} over $\mathbb{R}^{d_0} \times \{\pm 1\}$.
- \mathcal{D} can be separated by an invariant classifier β_0 .



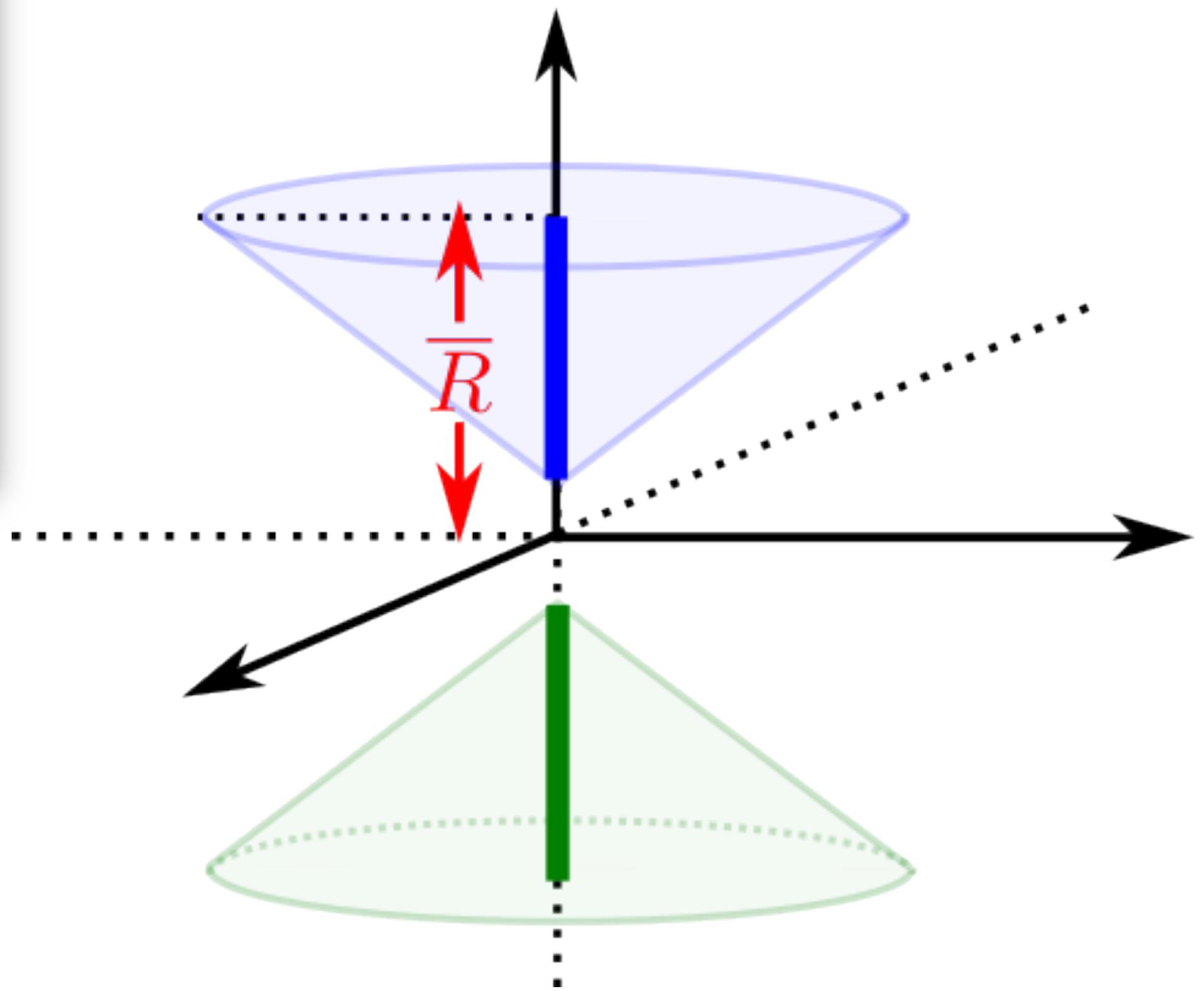
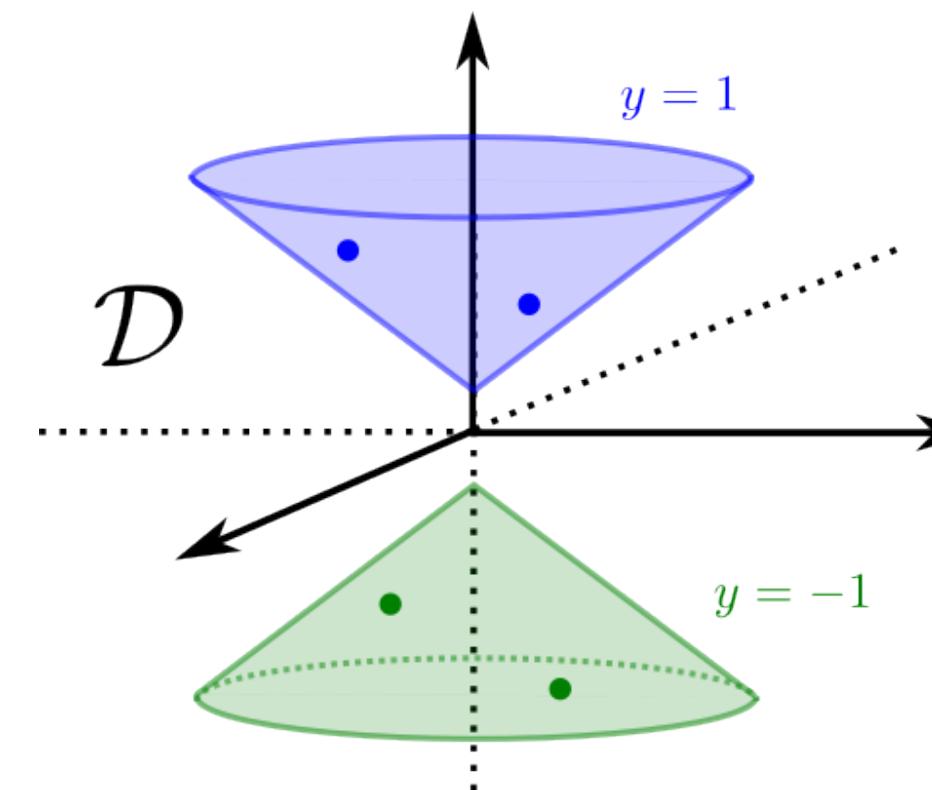
Improved generalization

- G -invariant distribution \mathcal{D} over $\mathbb{R}^{d_0} \times \{\pm 1\}$.
- \mathcal{D} can be separated by an invariant classifier β_0 .

Theorem [Chen and Z., NeurIPS 2023]

Let $\bar{R} = \inf \{r > 0 : \|\bar{\mathbf{x}}\| \leq r\}$. For any $\delta > 0$, w.p. at least $1 - \delta$,

$$\mathbb{P}_{(\mathbf{x},y) \sim \mathcal{D}} \left[y \neq \text{sign} \left(\langle \mathbf{x}, \beta_{\text{inv}}^\infty \rangle \right) \right] \leq \frac{2\bar{R}\|\beta_0\|}{\sqrt{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}$$



Improved generalization

- G -invariant distribution \mathcal{D} over $\mathbb{R}^{d_0} \times \{\pm 1\}$.
- \mathcal{D} can be separated by an invariant classifier β_0 .

Theorem [Chen and Z., NeurIPS 2023]

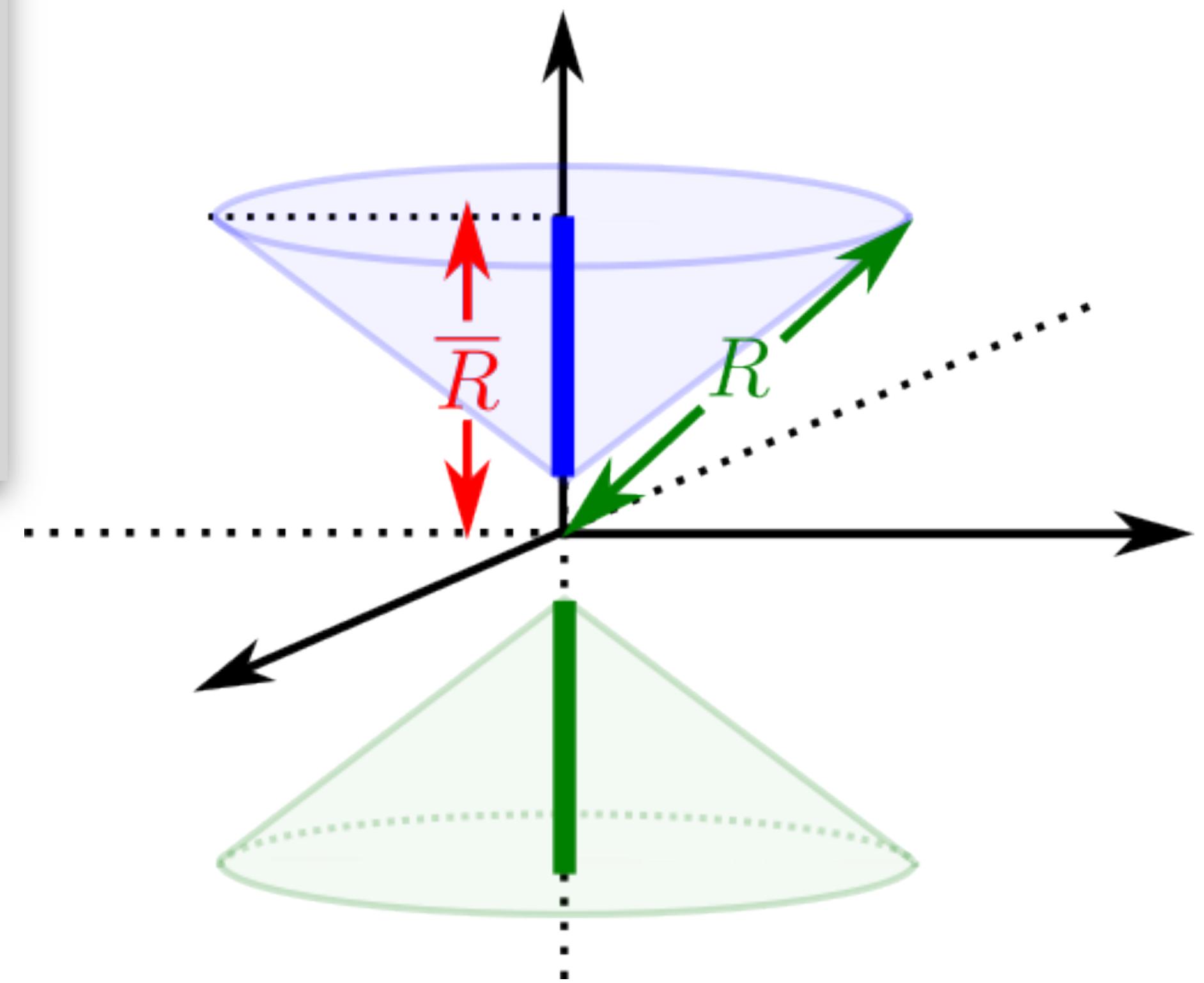
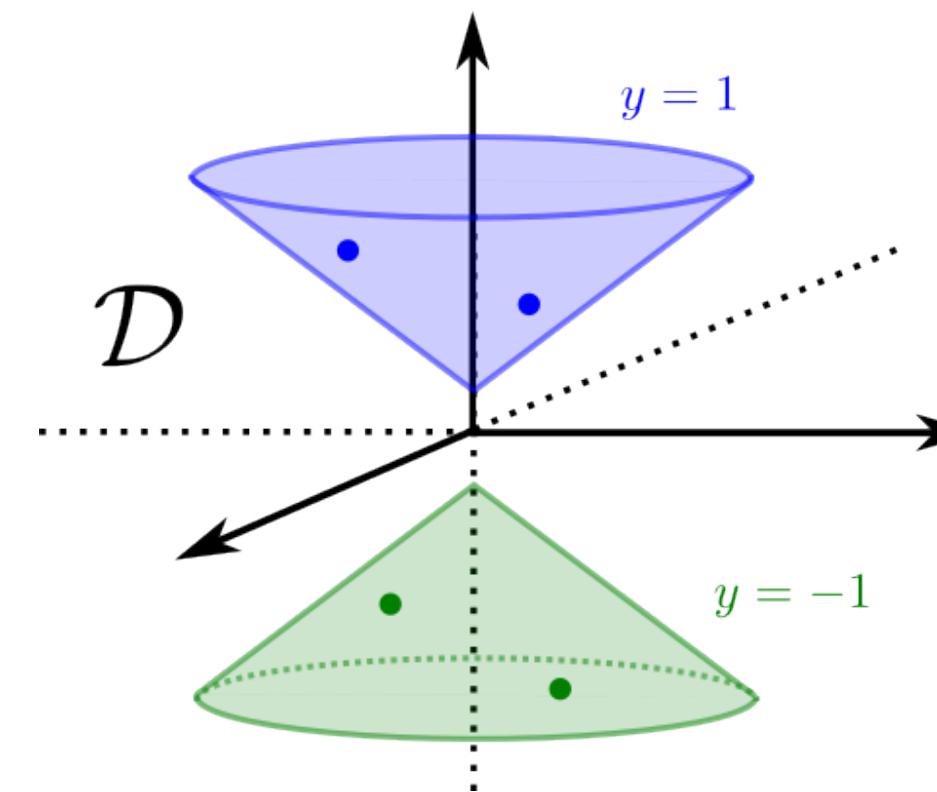
Let $\bar{R} = \inf \{r > 0 : \|\bar{\mathbf{x}}\| \leq r\}$. For any $\delta > 0$, w.p. at least $1 - \delta$,

$$\mathbb{P}_{(\mathbf{x},y) \sim \mathcal{D}} \left[y \neq \text{sign} \left(\langle \mathbf{x}, \beta_{\text{inv}}^\infty \rangle \right) \right] \leq \frac{2\bar{R}\|\beta_0\|}{\sqrt{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}$$

Remark: In comparison, for fully-connected networks, we have

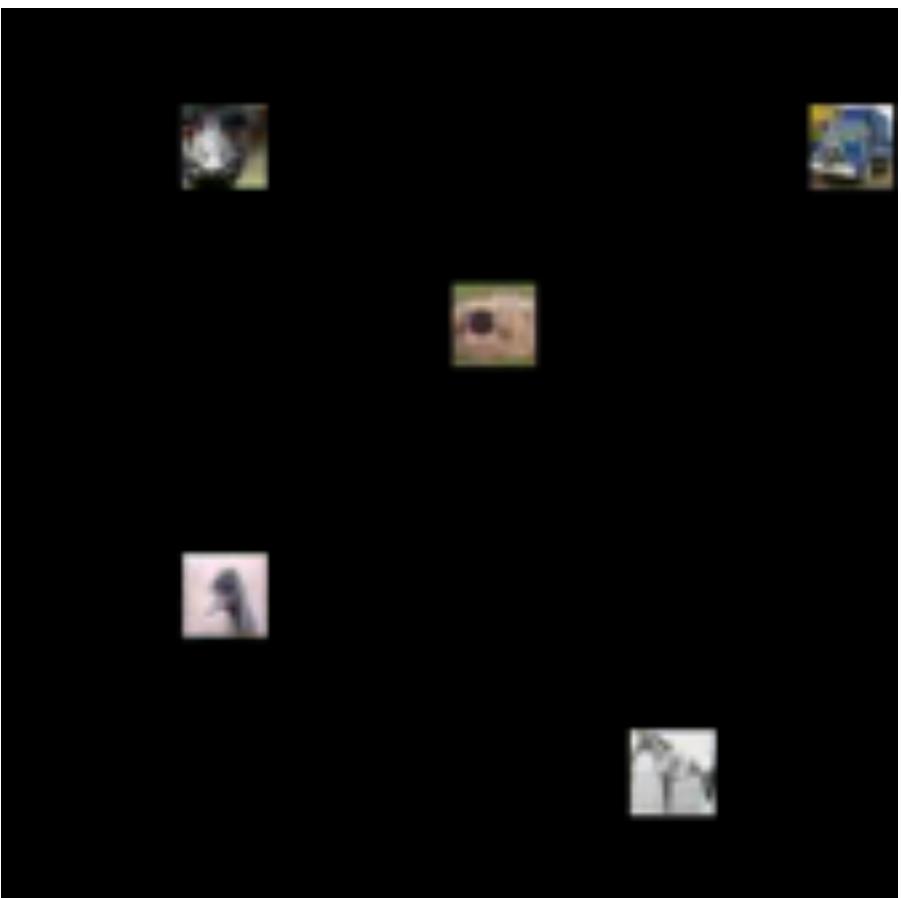
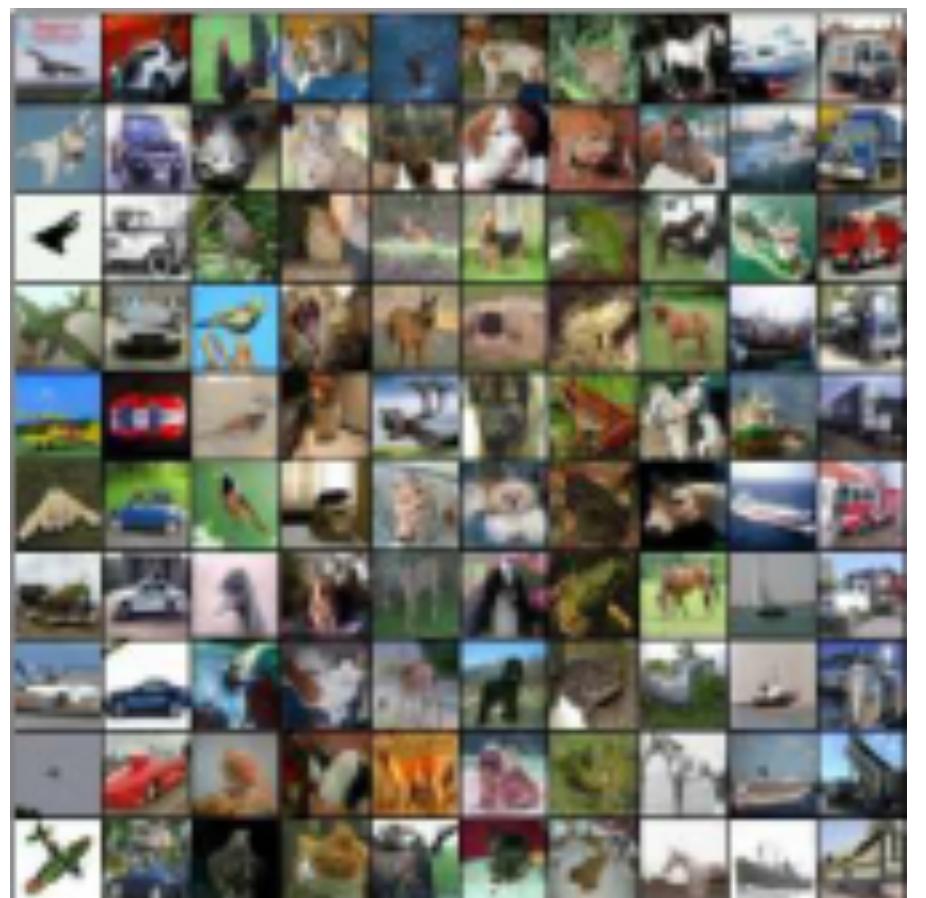
$$\mathbb{P}_{(\mathbf{x},y) \sim \mathcal{D}} \left[y \neq \text{sign} \left(\langle \mathbf{x}, \beta_{\text{fc}}^\infty \rangle \right) \right] \leq \frac{2R\|\beta_0\|}{\sqrt{n}} + \sqrt{\frac{\log(1/\delta)}{2n}},$$

where $R = \inf \{r > 0 : \|\mathbf{x}\| \leq r \text{ with probability } 1\} \geq \bar{R}$



Conclusion

- Exact quantification of the improvement
 - Sample complexity and error bound.
- Does it converge? To what solution?
 - Training dynamics of equivariant models



$$\mathbf{W}^* = \arg \min_{\mathbf{W}} \mathcal{L}(\mathbf{W}; S) = \sum_{i=1}^n \ell(f(\mathbf{x}_i; \mathbf{W}), y_i)$$

Related papers

- J. Birrell, M.A. Katsoulakis, L. Rey-Bellet, **W. Zhu**. “Structure-preserving GANs”. *ICML* (2022)
- Z. Chen, M.A. Katsoulakis, L. Rey-Bellet, **W. Zhu**. “Sample complexity of probability divergences under group symmetry”. *ICML* (2023)
- Z. Chen and **W. Zhu**. “On the implicit bias of linear equivariant steerable networks: margin, generalization, and their equivalence to data augmentation”. *NeurIPS* (2023)

Acknowledgement

NSF DMS-2052525, DMS-2140982, and DMS-2244976.

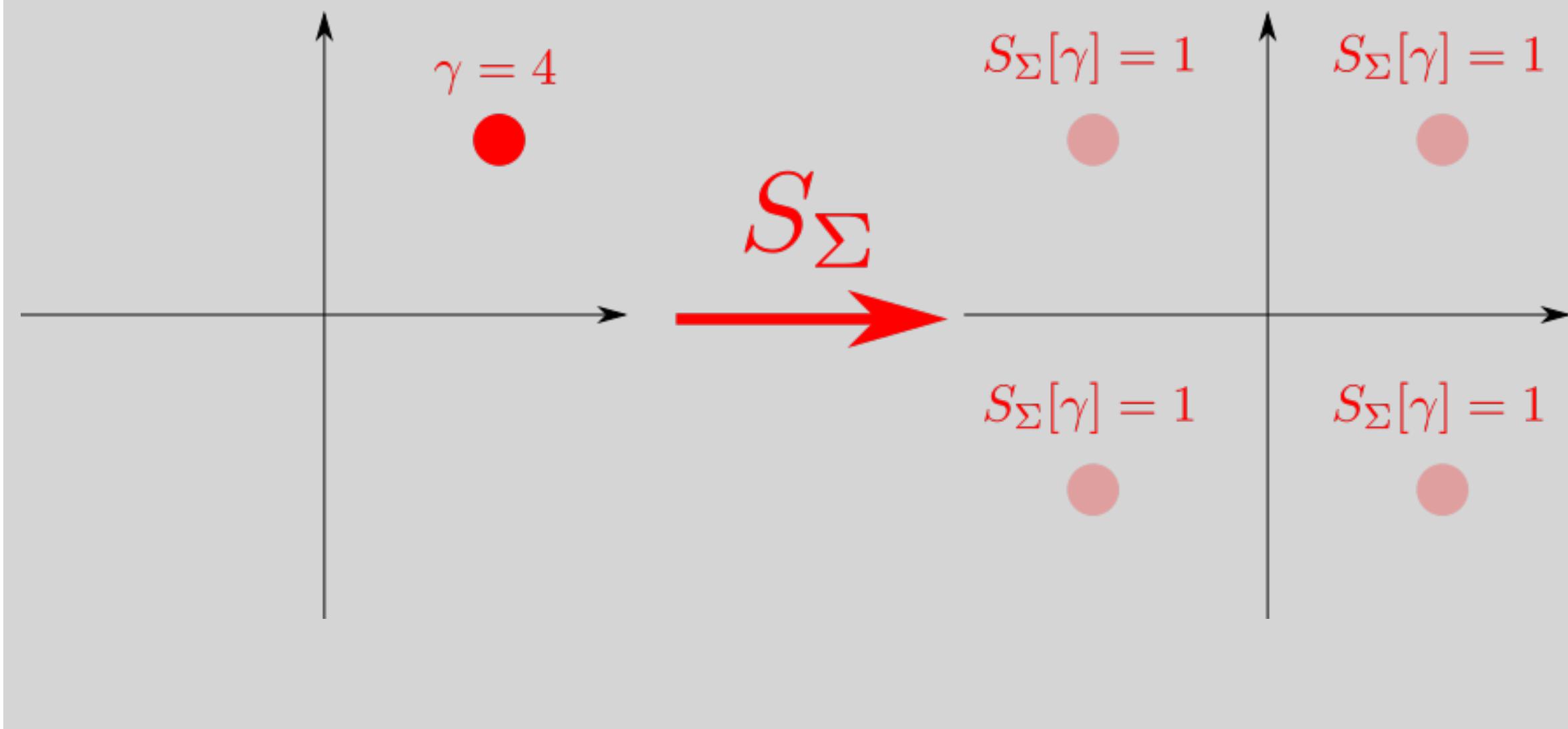


Symmetrization operators S_Σ and S^Σ

Symmetrization operators S_Σ and S^Σ

- Symmetrization of functions: $S_\Sigma : \mathcal{M}_b(X) \rightarrow \mathcal{M}_b(X)$,

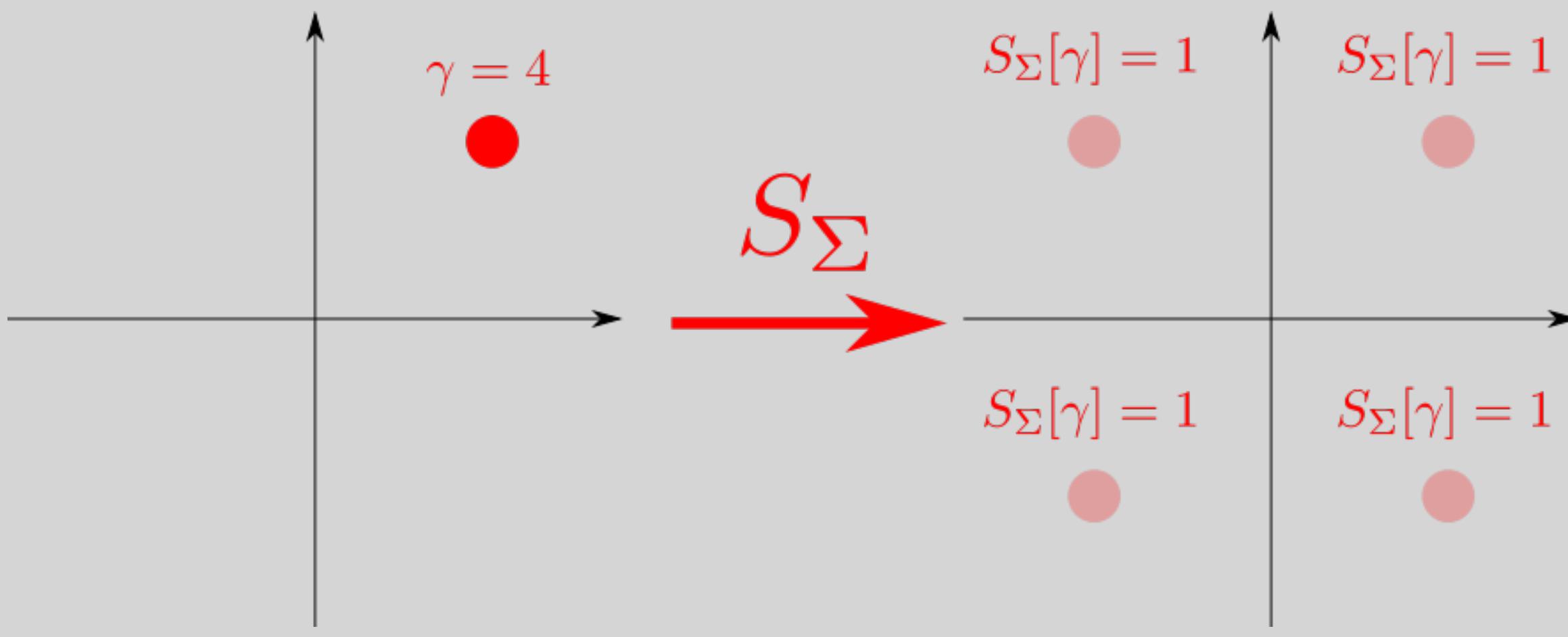
$$S_\Sigma[\gamma](x) = \int_{\Sigma} \gamma(T_\sigma(x)) \mu_\Sigma(d\sigma') = E_{\mu_\Sigma}[\gamma \circ T_\sigma(x)].$$



Symmetrization operators S_Σ and S^Σ

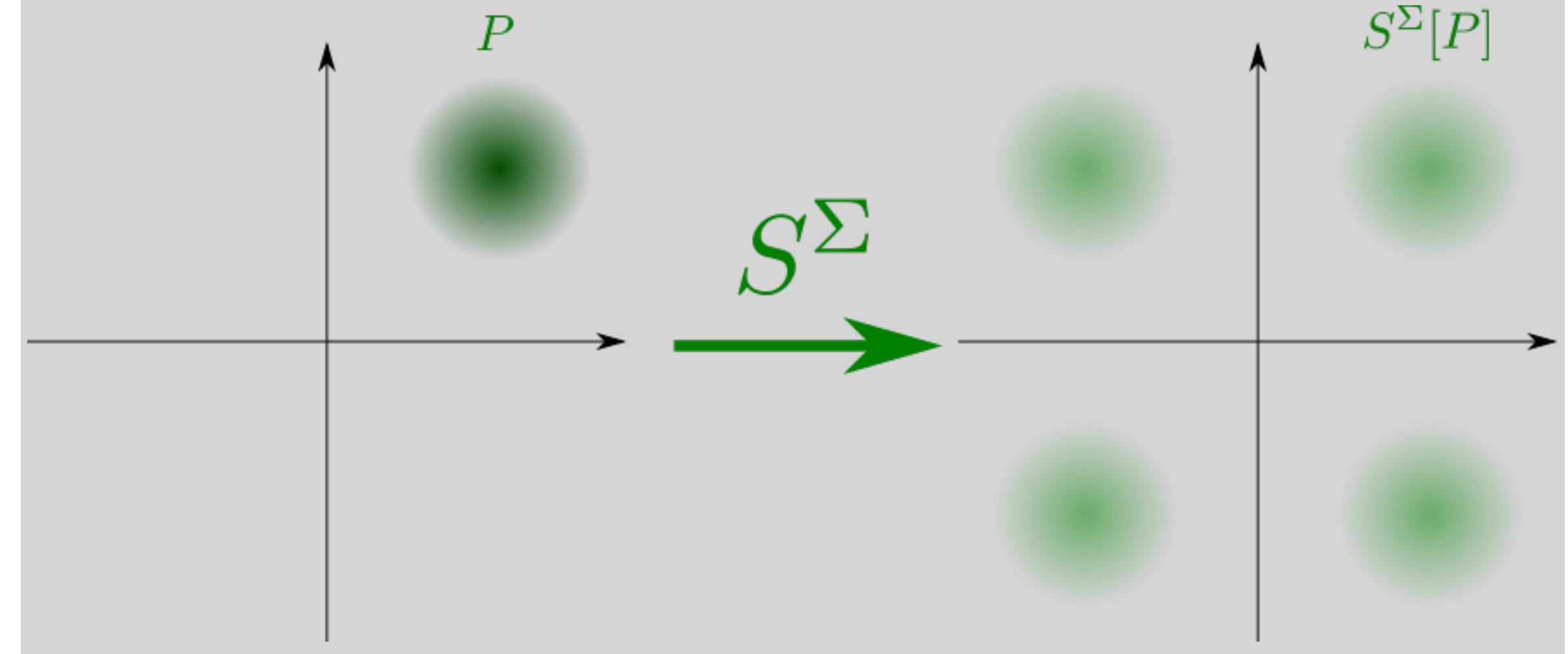
- Symmetrization of functions: $S_\Sigma : \mathcal{M}_b(X) \rightarrow \mathcal{M}_b(X)$,

$$S_\Sigma[\gamma](x) = \int_{\Sigma} \gamma(T_\sigma(x)) \mu_\Sigma(d\sigma') = E_{\mu_\Sigma}[\gamma \circ T_\sigma(x)].$$



- Symmetrization of measures: $S^\Sigma : \mathcal{P}(X) \rightarrow \mathcal{P}(X)$,

$$E_{S^\Sigma[P]} \gamma = \int_X S_\Sigma[\gamma](x) dP(x) = E_P S_\Sigma[\gamma], \forall \gamma \in \mathcal{M}_b(X).$$

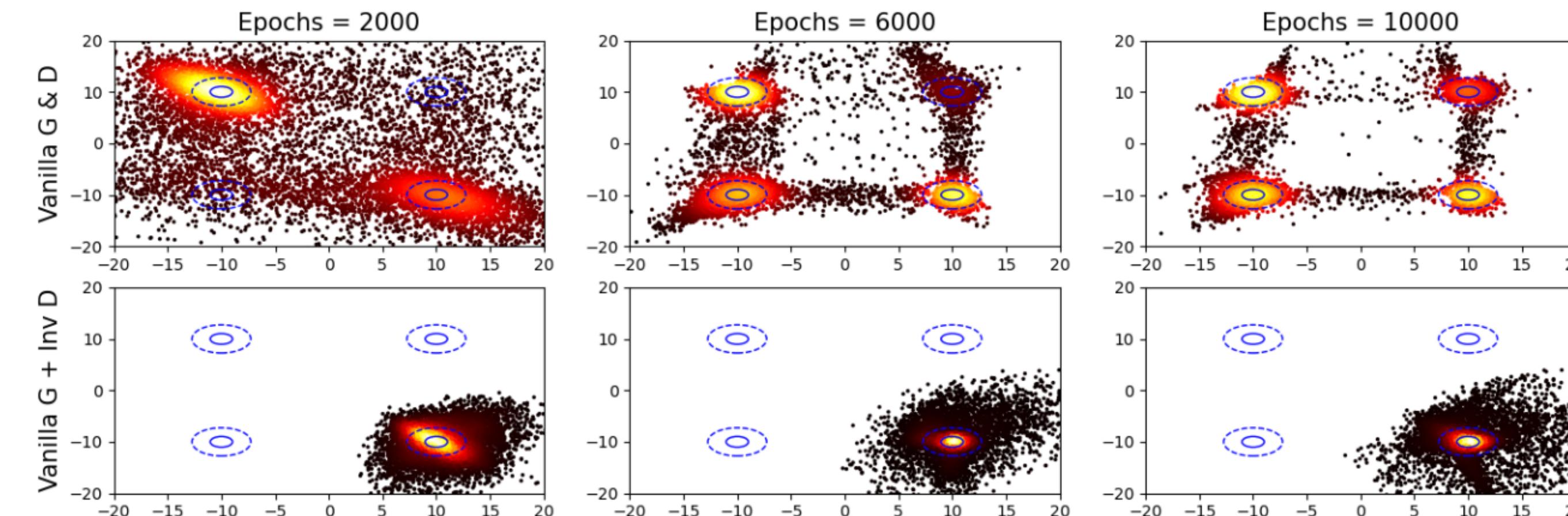


Mode collapse – a warning

Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

If $S_\Sigma[\Gamma] \subset \Gamma$ and $P, Q \in \mathcal{P}(X)$, i.e., **not necessarily Σ -invariant**, then

$$D^{\Gamma_\Sigma^{\text{inv}}}(Q||P) = D^\Gamma(S^\Sigma[Q]||S^\Sigma[P]).$$



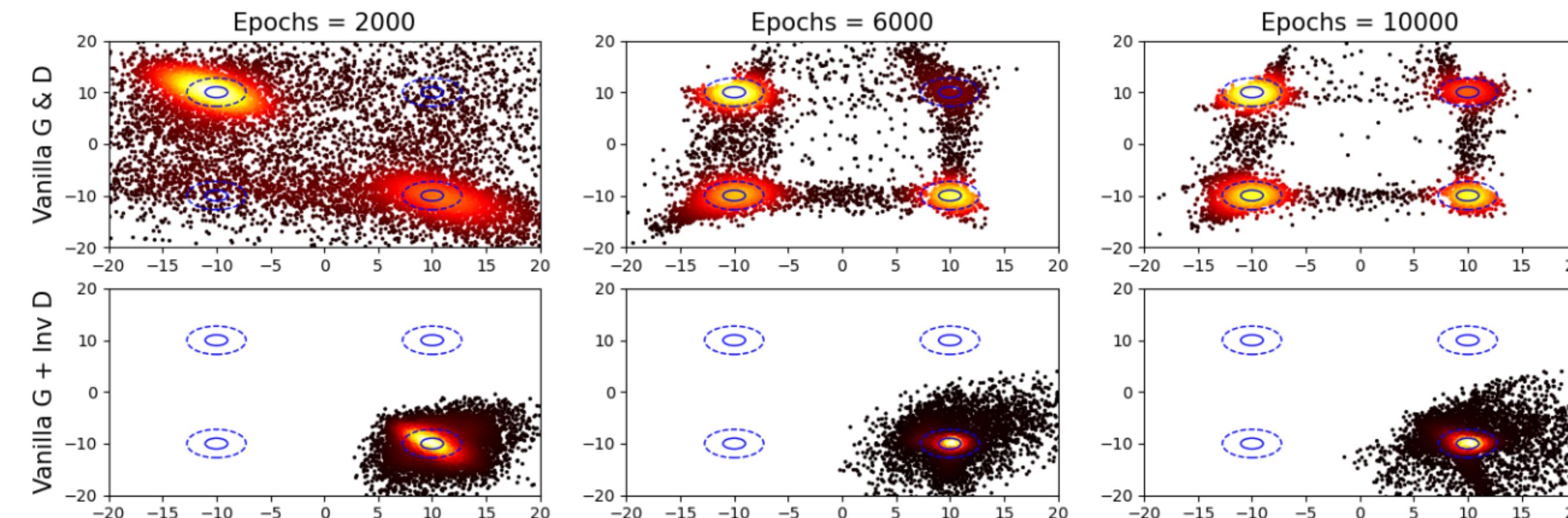
Mode collapse – a warning

Theorem [Birrell, Katsoulakis, Rey-Bellet, Z., ICML 2022]

If $S_\Sigma[\Gamma] \subset \Gamma$ and $P, Q \in \mathcal{P}(X)$, i.e., **not necessarily Σ -invariant**, then

$$D^{\Gamma_\Sigma^{\text{inv}}}(Q||P) = D^\Gamma(S^\Sigma[Q]||S^\Sigma[P]).$$

- Reducing Γ to $\Gamma_\Sigma^{\text{inv}}$ might result in “**mode collapse**” if P_g is **NOT** Σ -invariant



Mode collapse – a warning

Theorem [Birrell, Katsoulakis, Rey-Bellet, **Z.**, ICML 2022]

If $S_\Sigma[\Gamma] \subset \Gamma$ and $P, Q \in \mathcal{P}(X)$, i.e., **not necessarily Σ -invariant**, then

$$D^{\Gamma_\Sigma^{\text{inv}}}(Q||P) = D^\Gamma(S^\Sigma[Q]||S^\Sigma[P]).$$

- Reducing Γ to $\Gamma_\Sigma^{\text{inv}}$ might result in “**mode collapse**” if P_g is **NOT** Σ -invariant
- The reason is as P_g only needs to equal Q after Σ -symmetrization.

