

Structure-Preserving GANs

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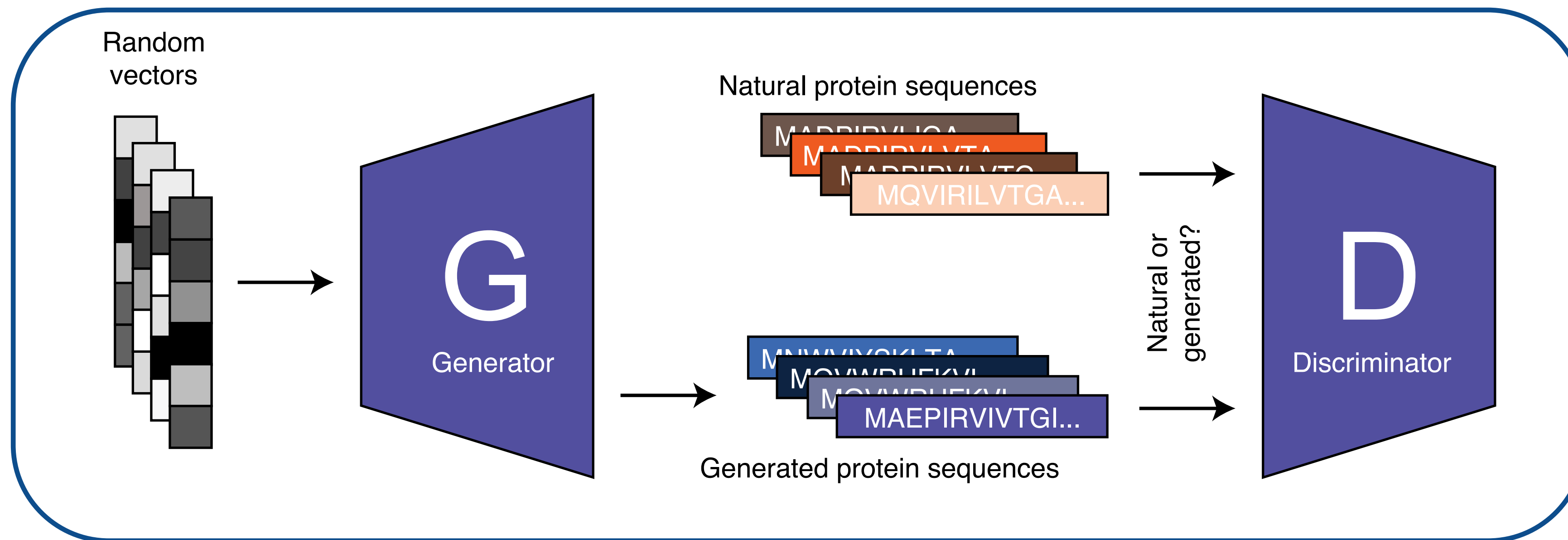


Figure: Repecka et al., *Nature Machine Intelligence* 2021

Generative adversarial networks (GANs)

- GANs use a pair of neural networks to **learn a 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.

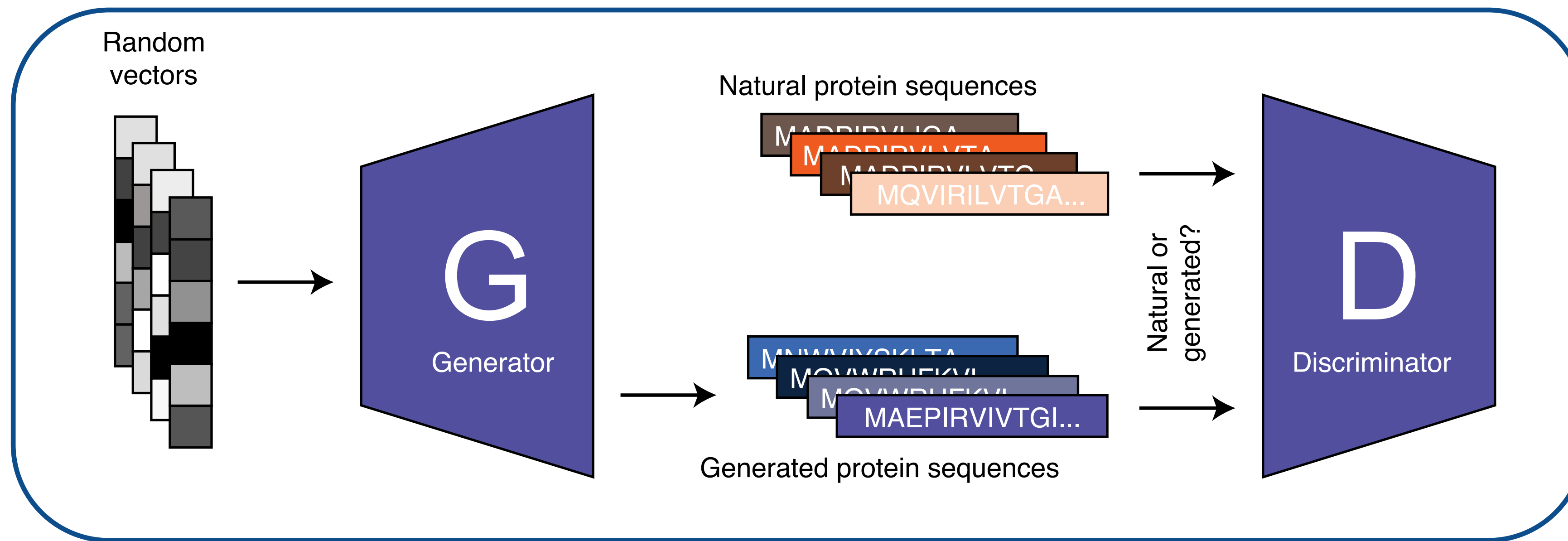
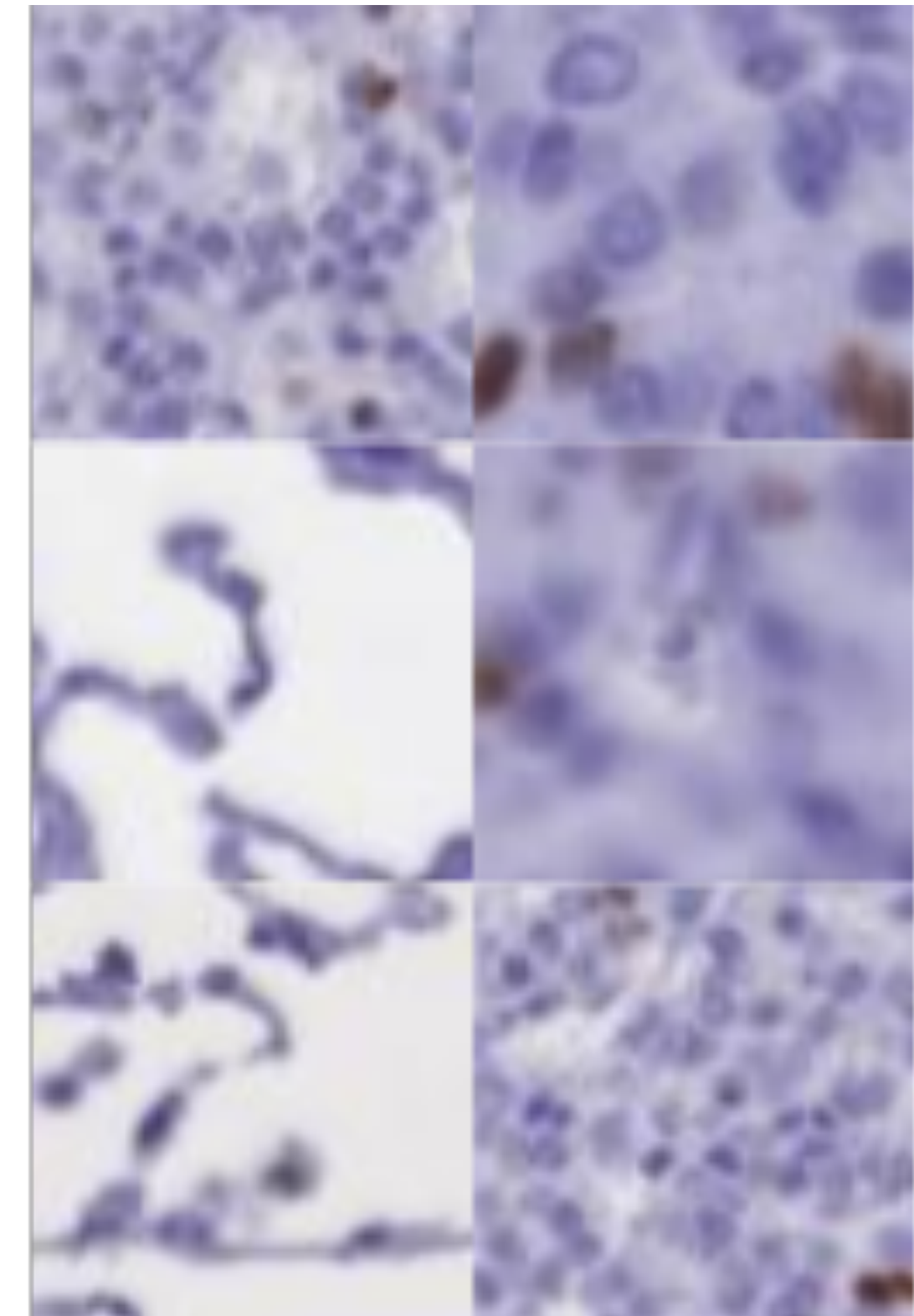
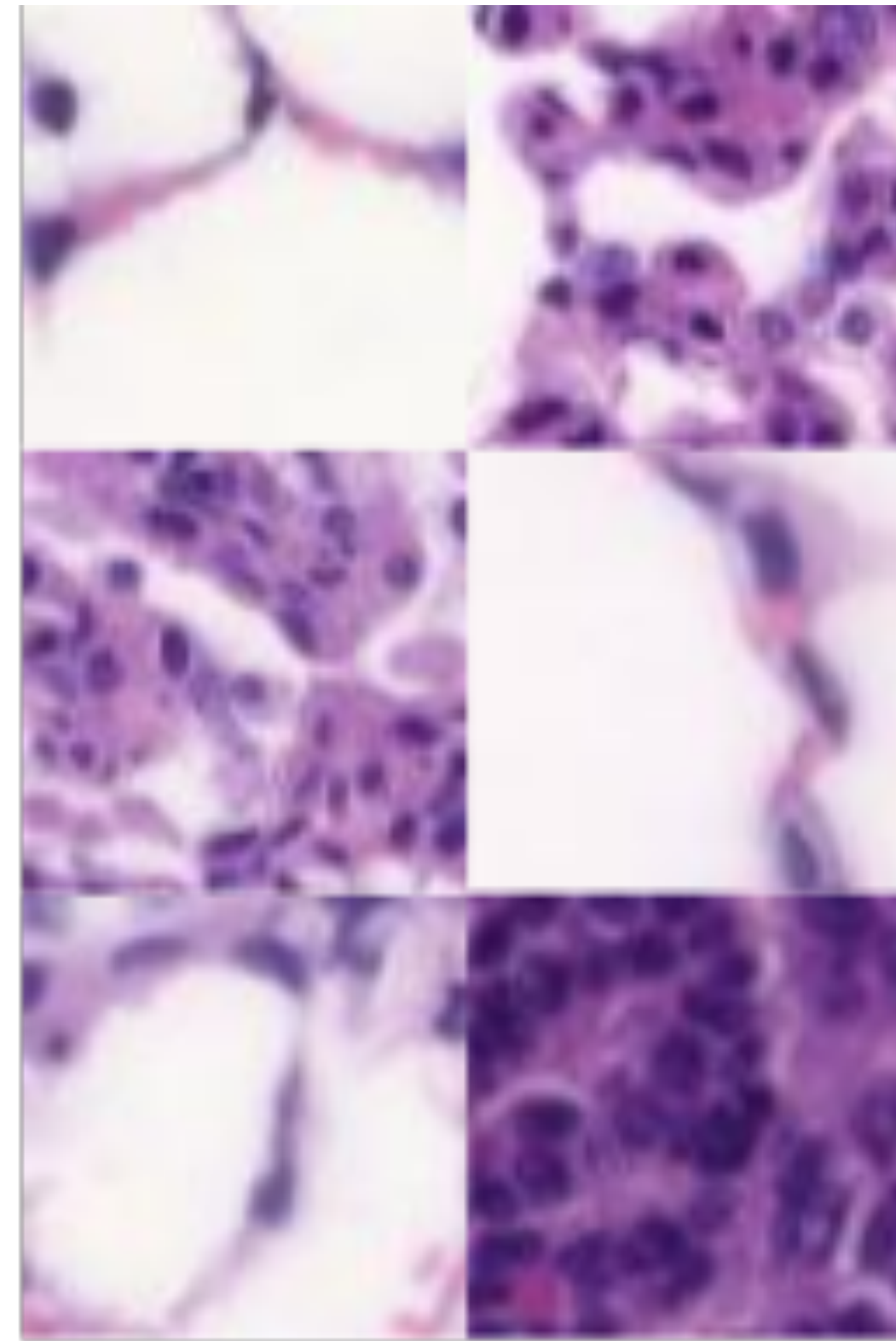
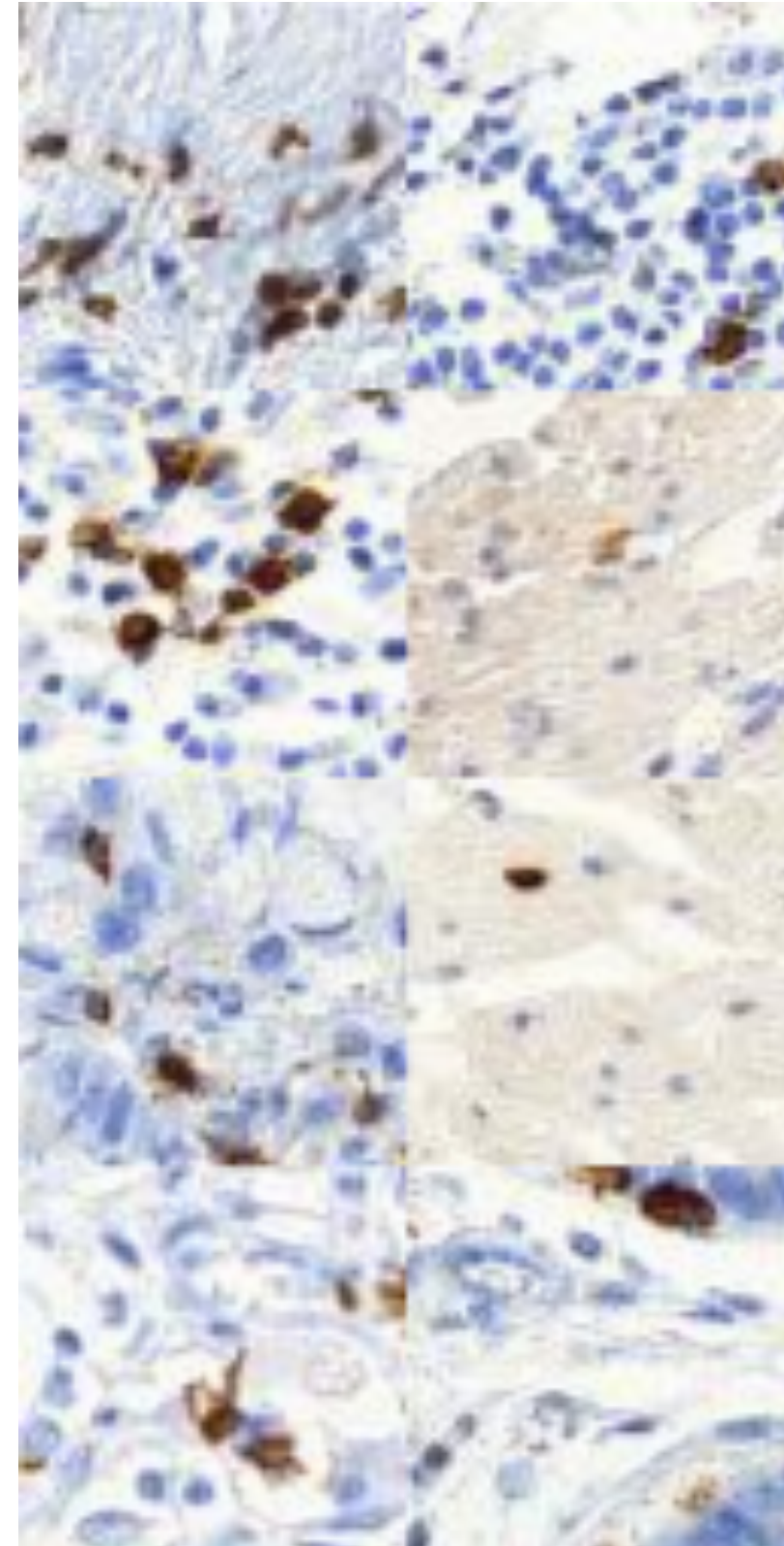
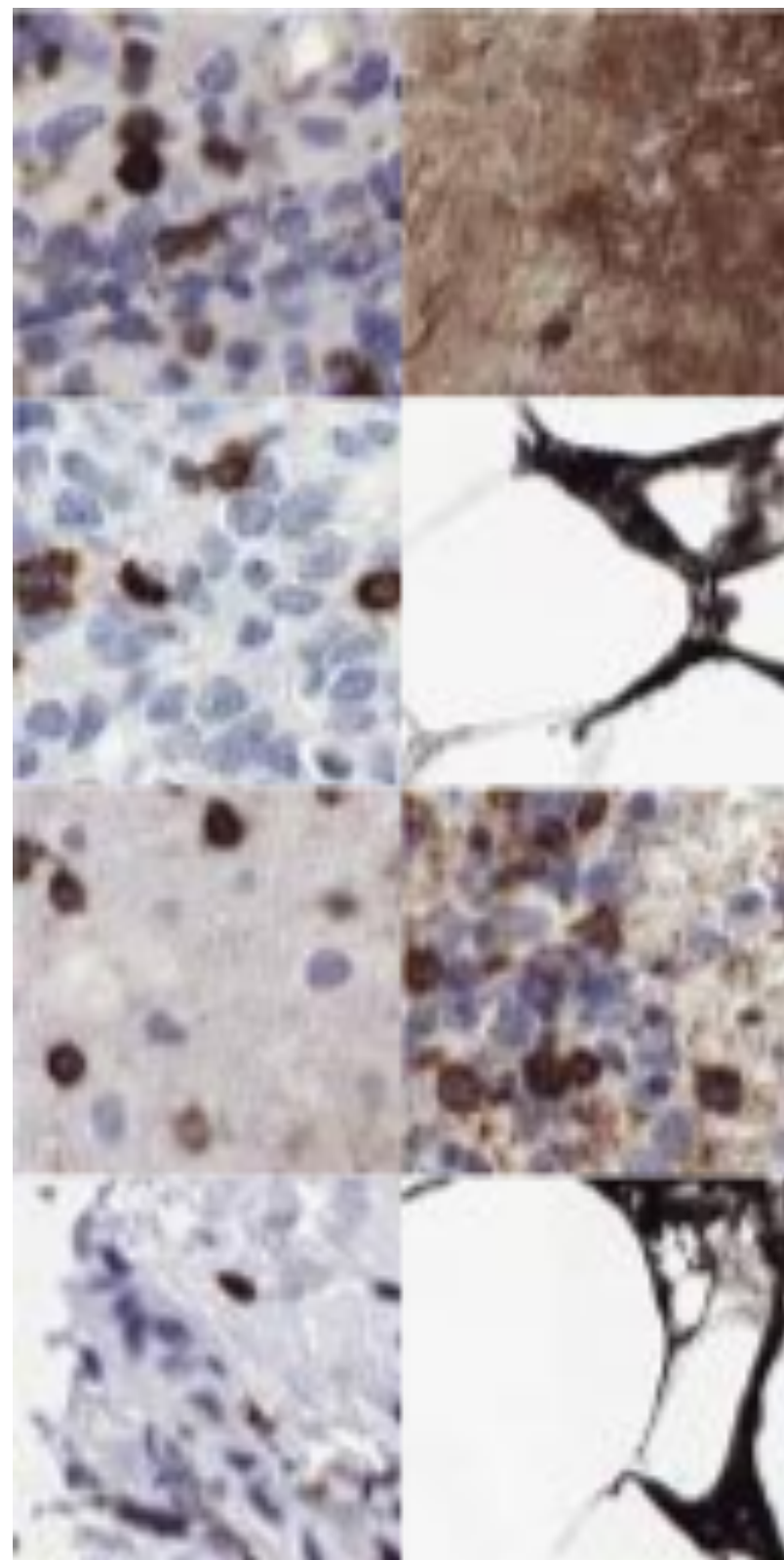


Figure: Repecka et al., *Nature Machine Intelligence* 2021

Structured target data & distribution Q

Q



LYSTO¹

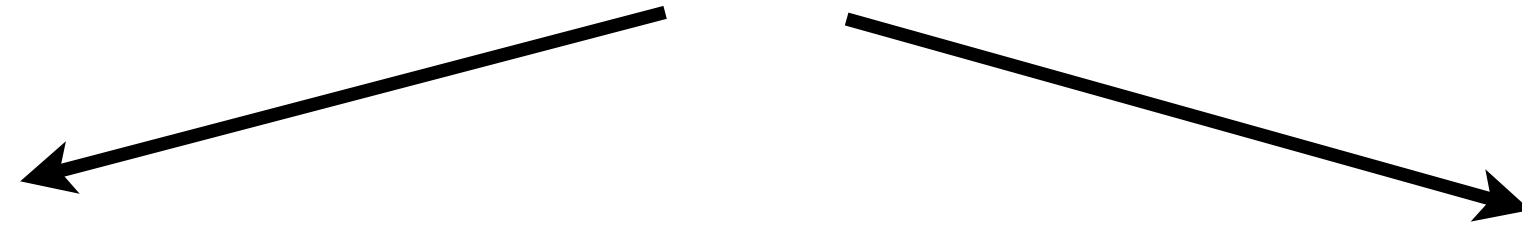
ANHIR²

1. Ciompi et al., Zenodo 2019

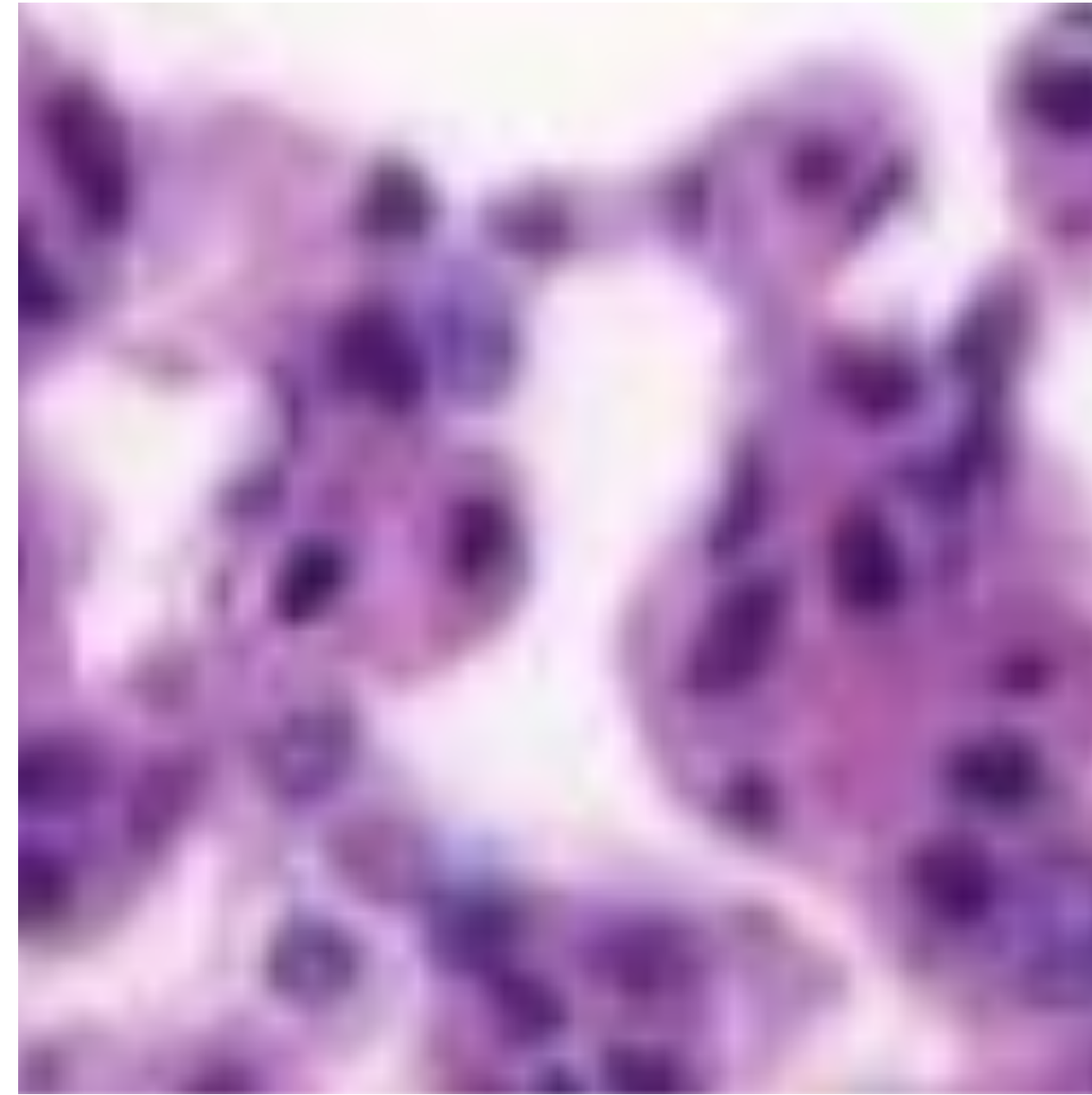
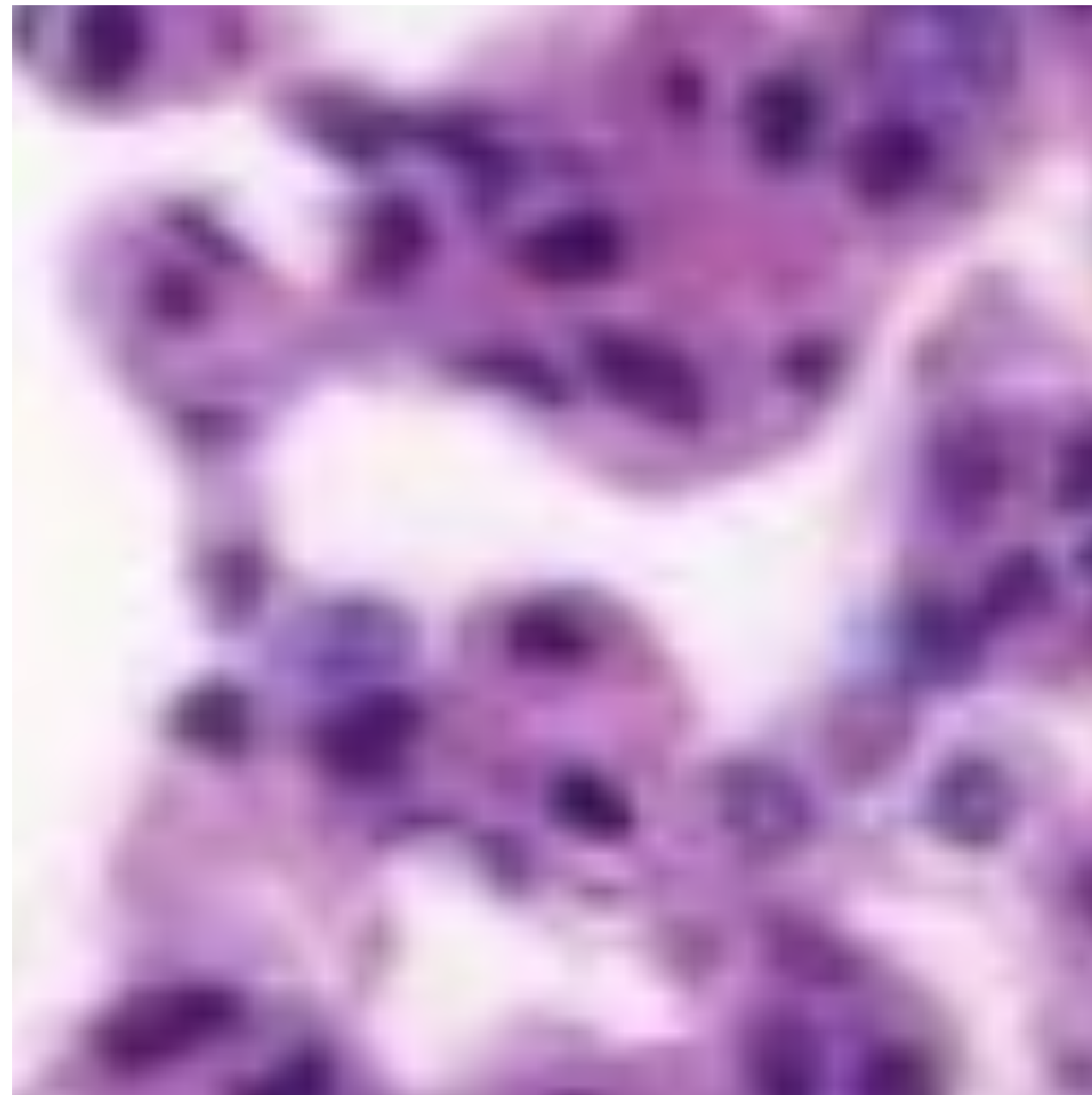
2. Borovec et al., IEEE Transactions on Medical Imaging 2020

Structured target data & distribution Q

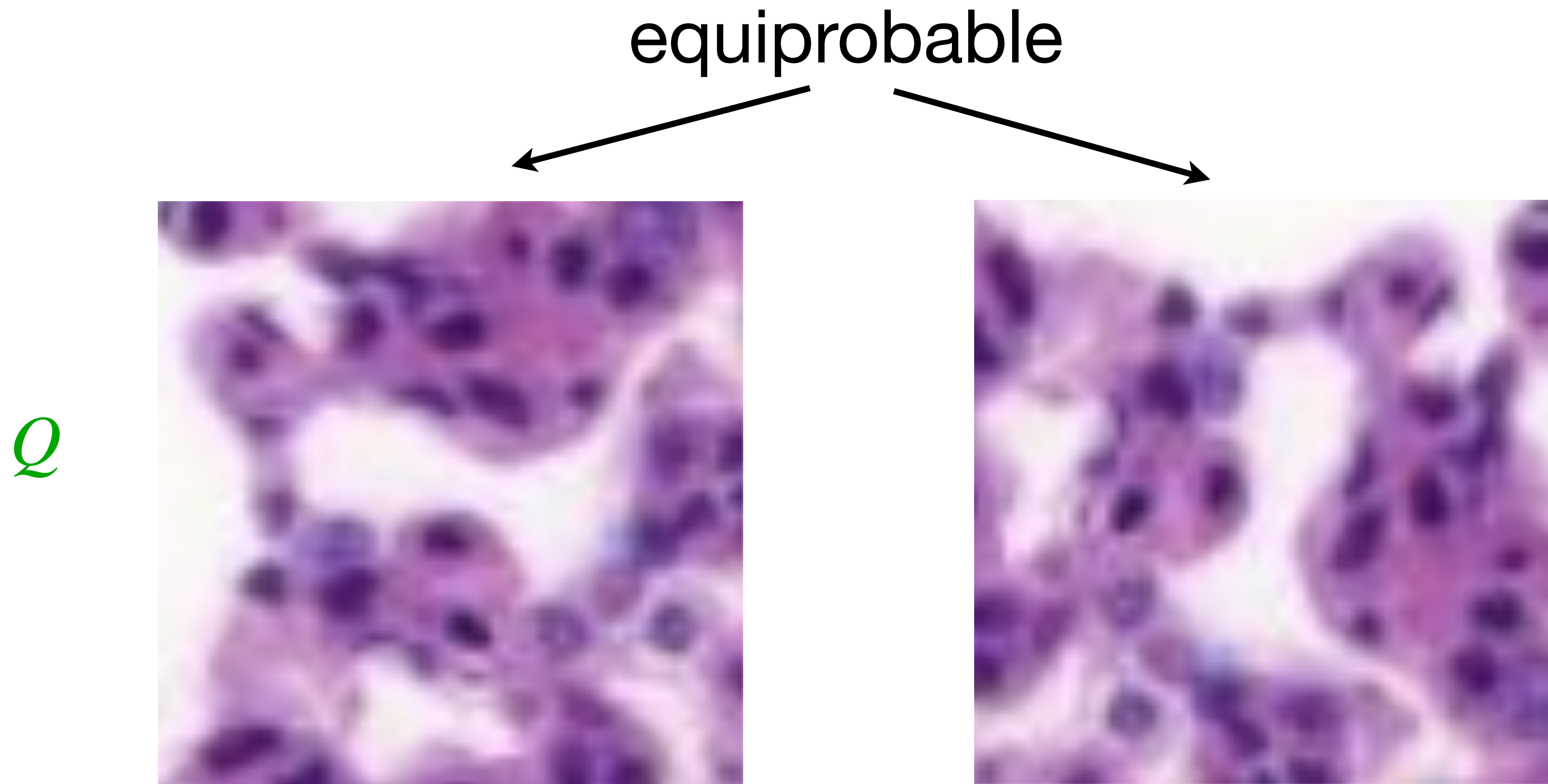
equiprobable



Q

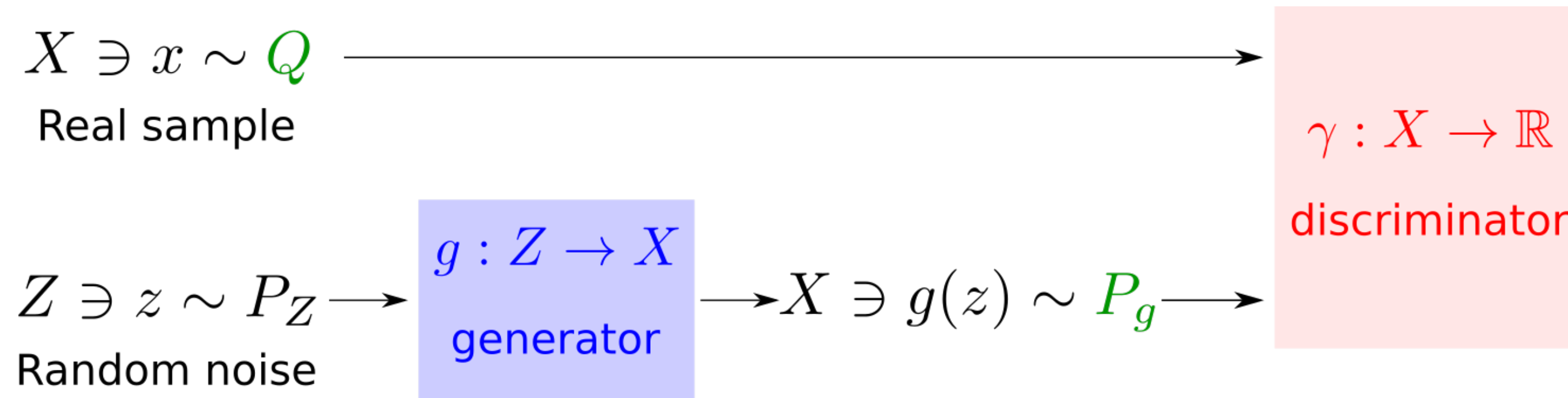


Structured target data & distribution Q



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

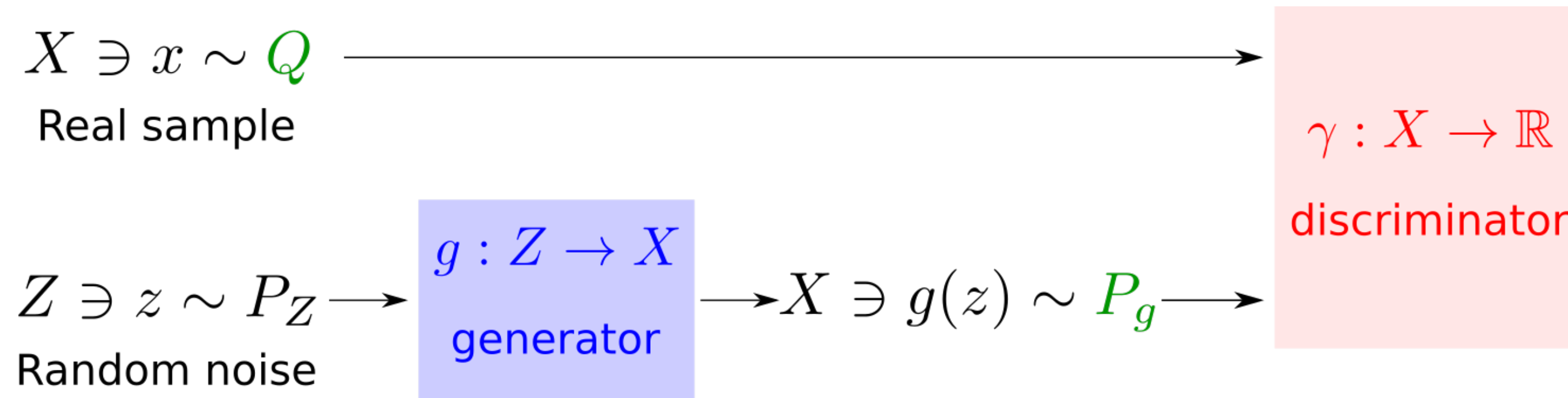
GAN is “probability distance” minimization



Mathematically, GANs can be formulated as minimizing some **variational divergence**, $D^\Gamma(Q \| P_g)$, between Q and P_g .

$$\min_{g \in G} D^\Gamma(Q \| P_g)$$

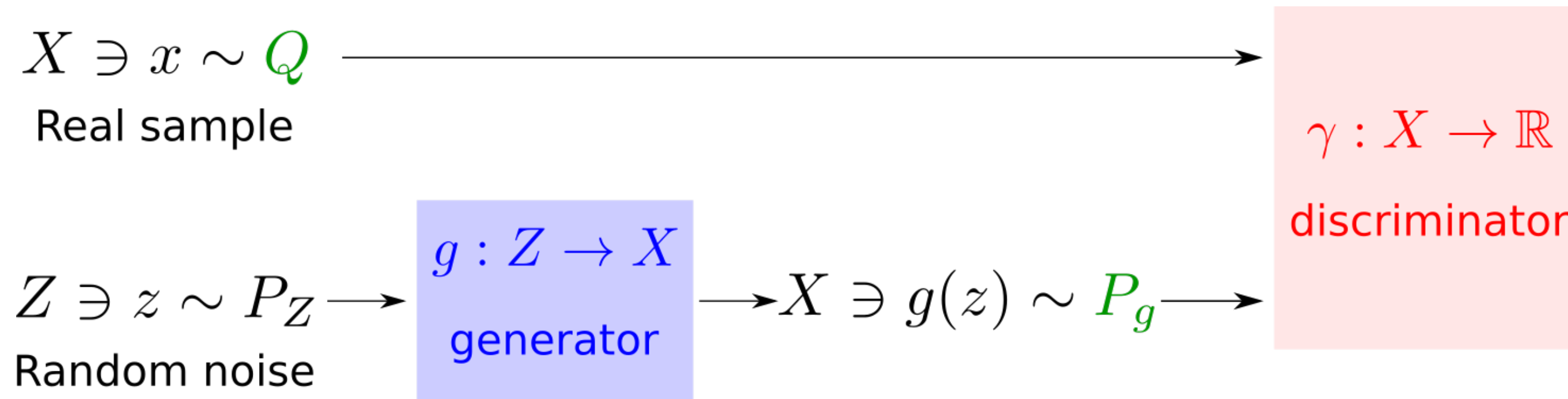
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Mathematically, GANs can be formulated as minimizing some **variational divergence**, $D^\Gamma(Q \| P_g)$, between Q and P_g . “Distance” is determined by **discriminators** $\gamma \in \Gamma$.

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

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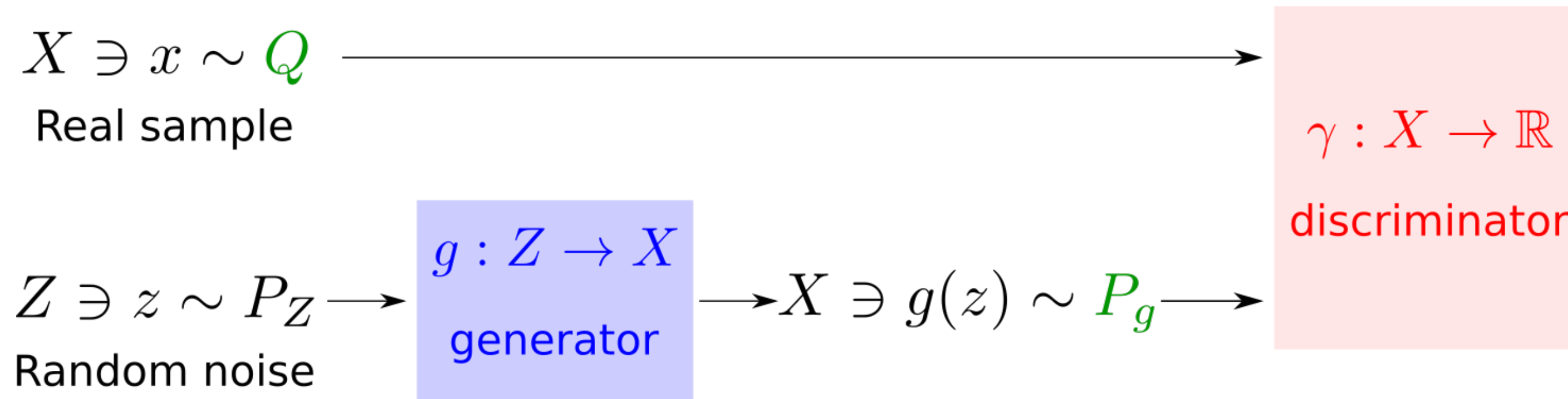


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- The original GAN [Goodfellow et al., 2014]: $\min_{g \in G} \max_{\gamma \in \Gamma} E_Q[\log \gamma] + E_{P_g}[\log(1 - \gamma)]$

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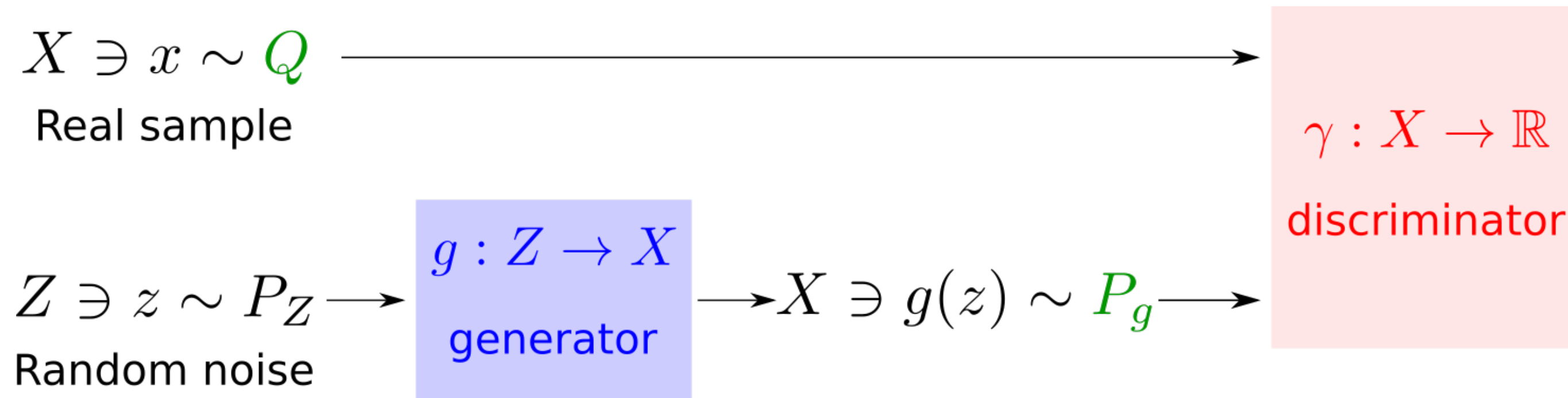


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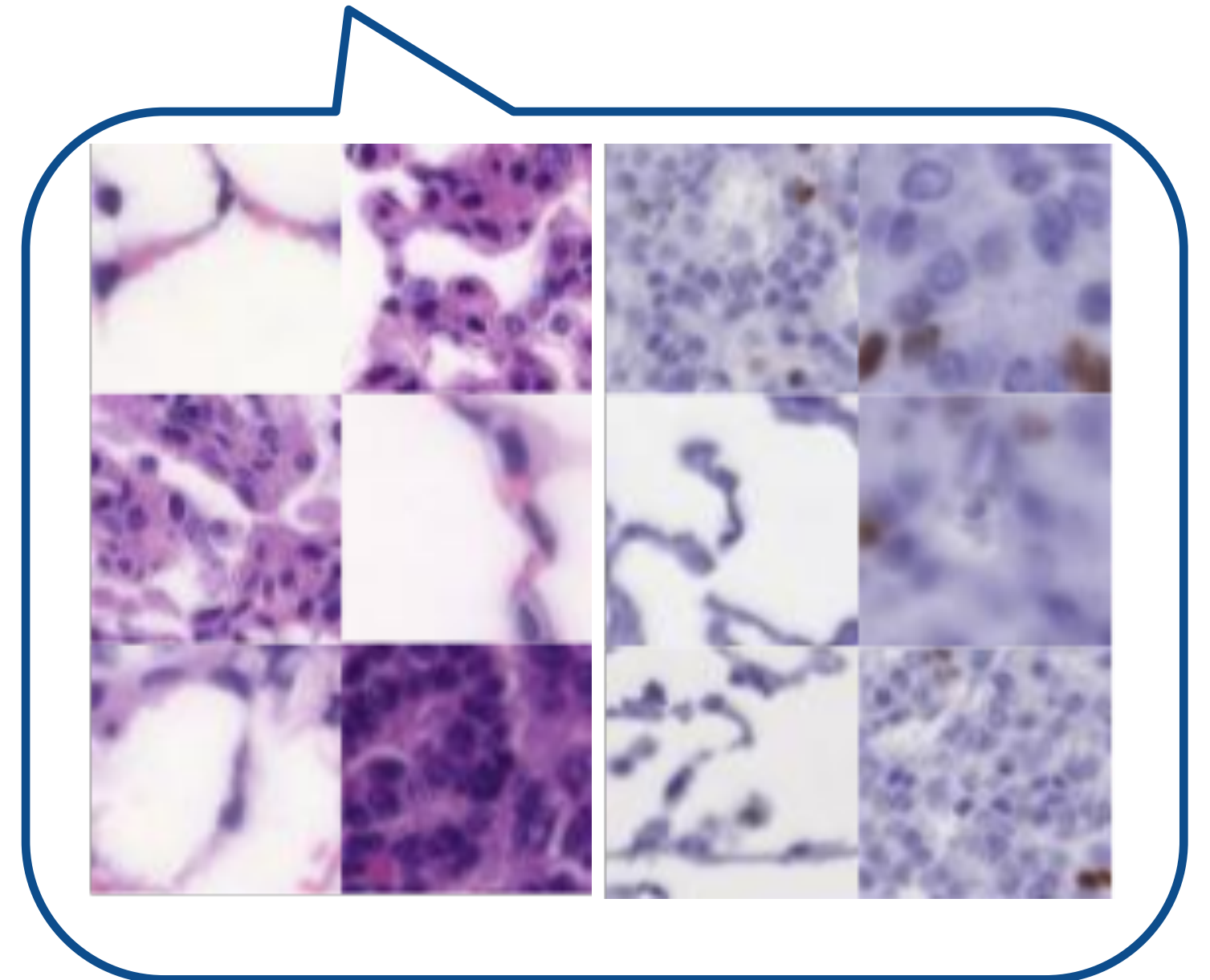
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- The original GAN [Goodfellow et al., 2014]: $\min_{g \in G} \max_{\gamma \in \Gamma} E_Q[\log \gamma] + E_{P_g}[\log(1 - \gamma)]$
- Many other variational divergences: KL, f-divergences, Wasserstein, MMD, Sinkhorn...

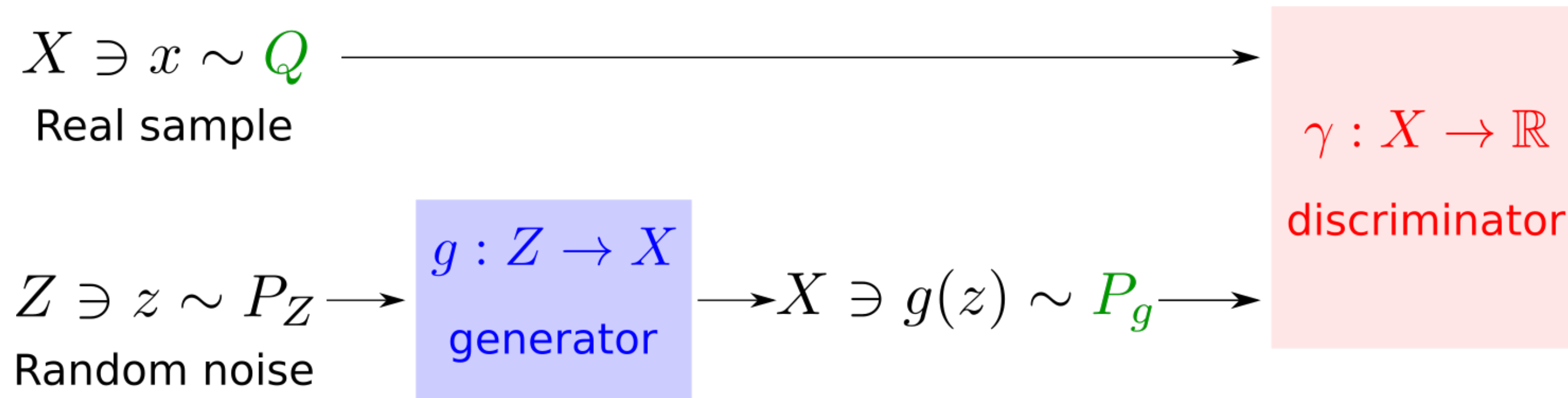
GAN with embedded structure



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

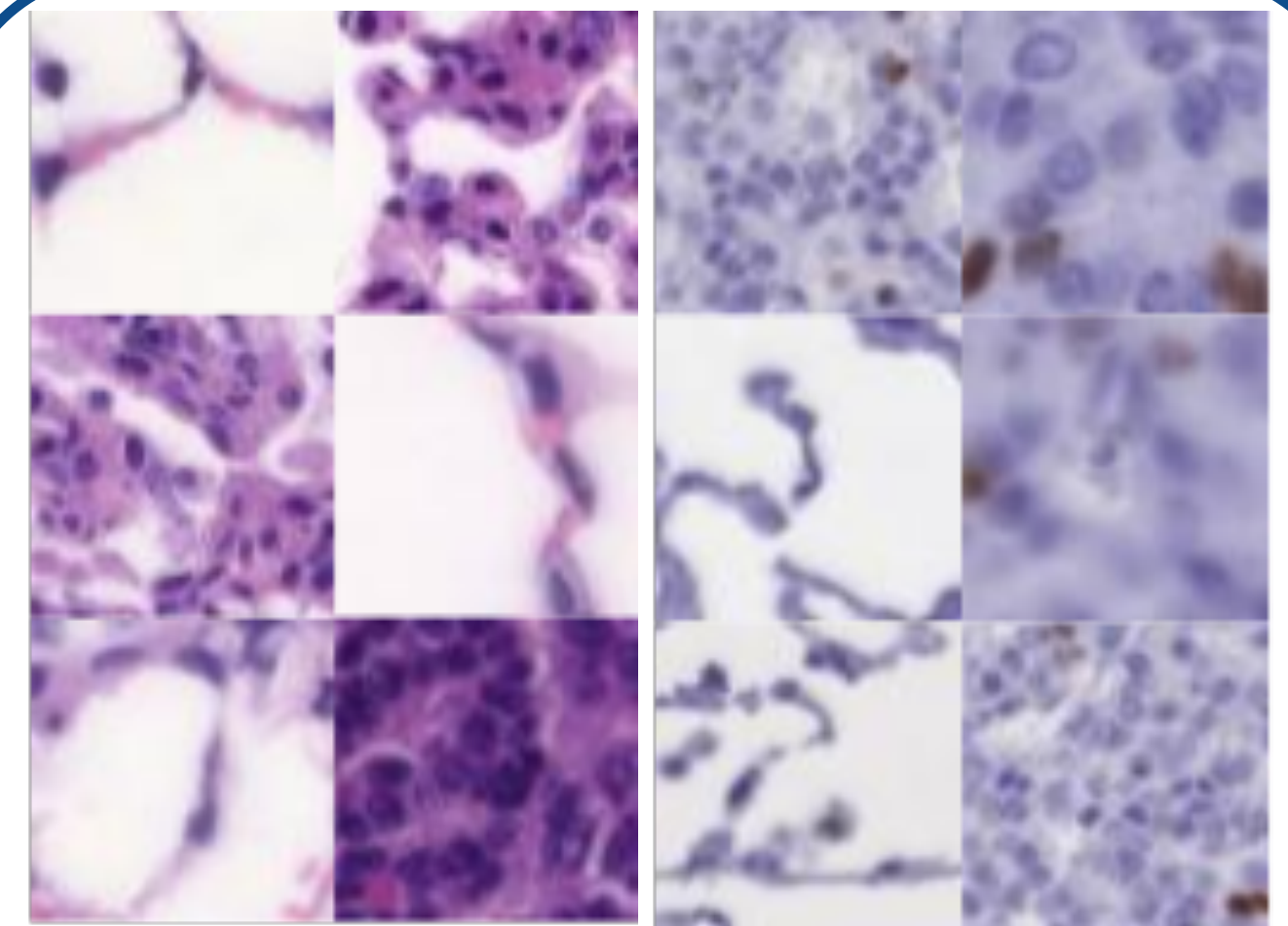


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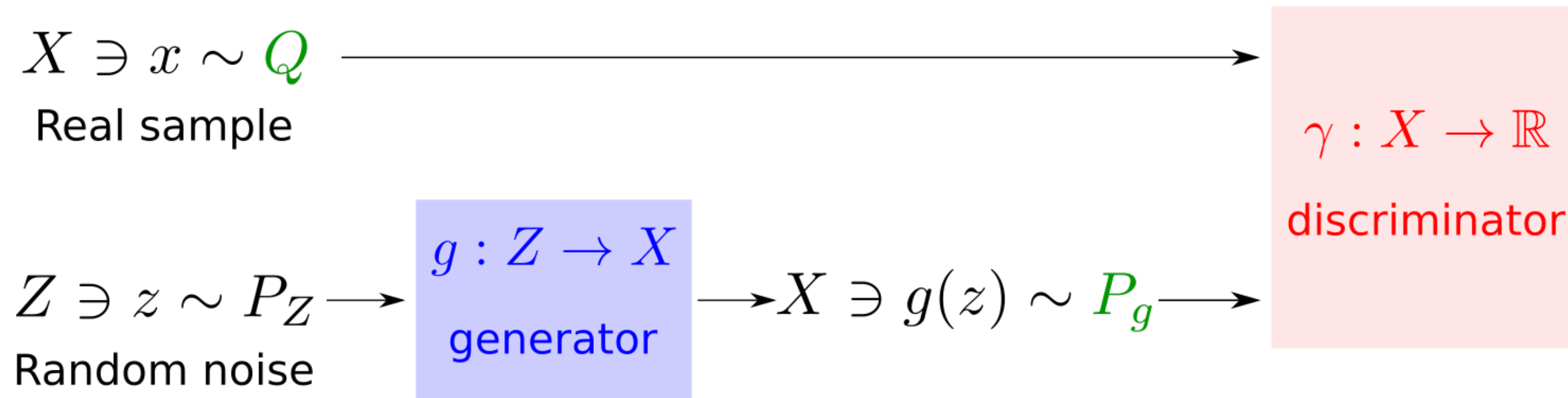


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- Σ : rotation, translation, roto-reflection, permutation, etc.

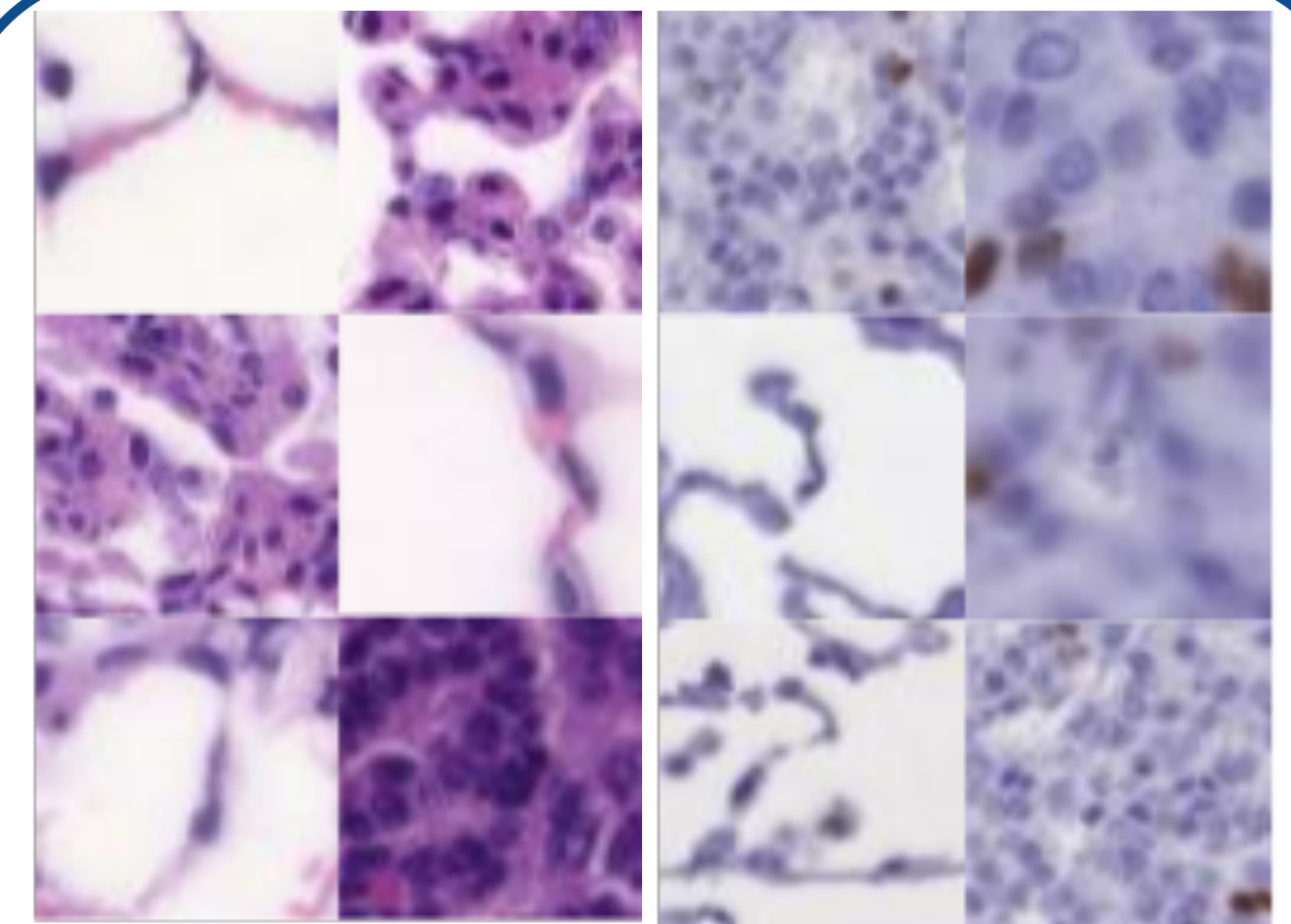


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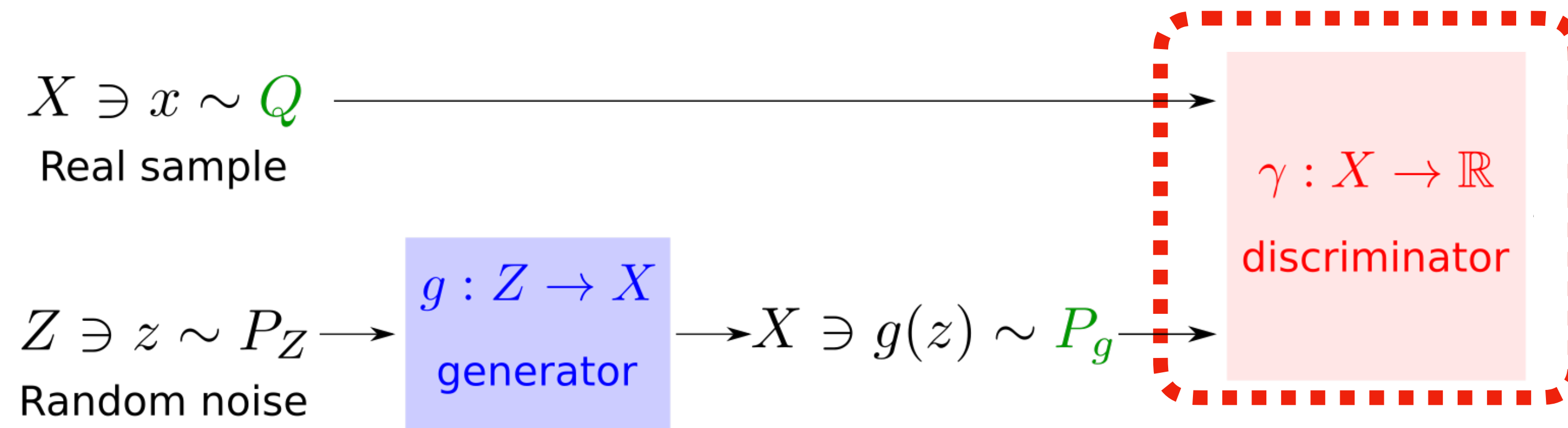


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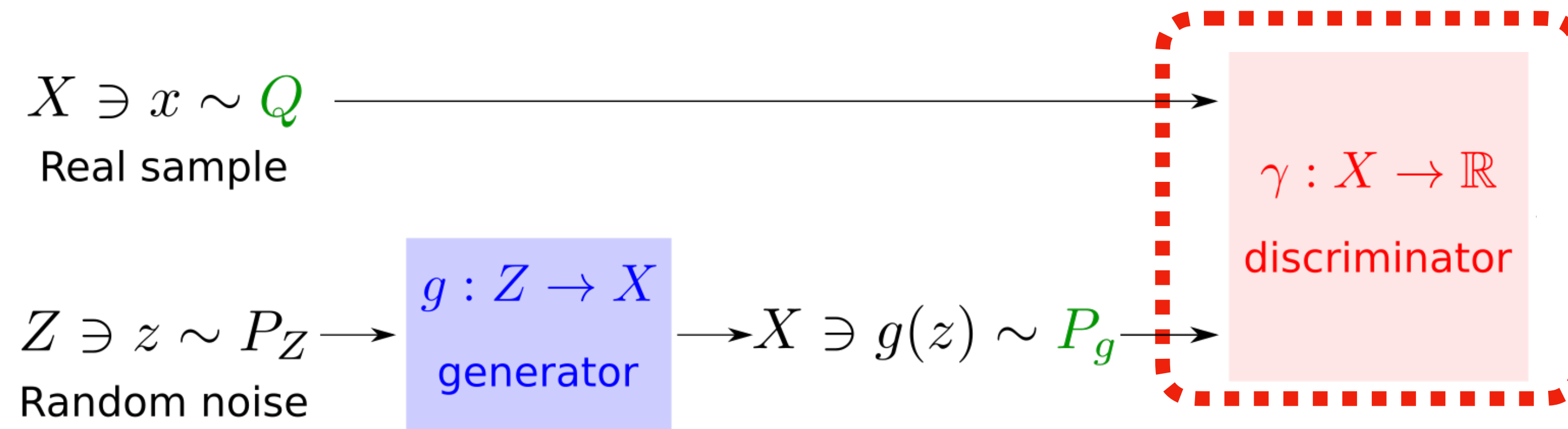
- Target distribution Q is invariant under a group Σ .
- Σ : rotation, translation, roto-reflection, permutation, etc.
- How to incorporate structure into g and γ ?



Our Theorem 1: “smarter” discriminator



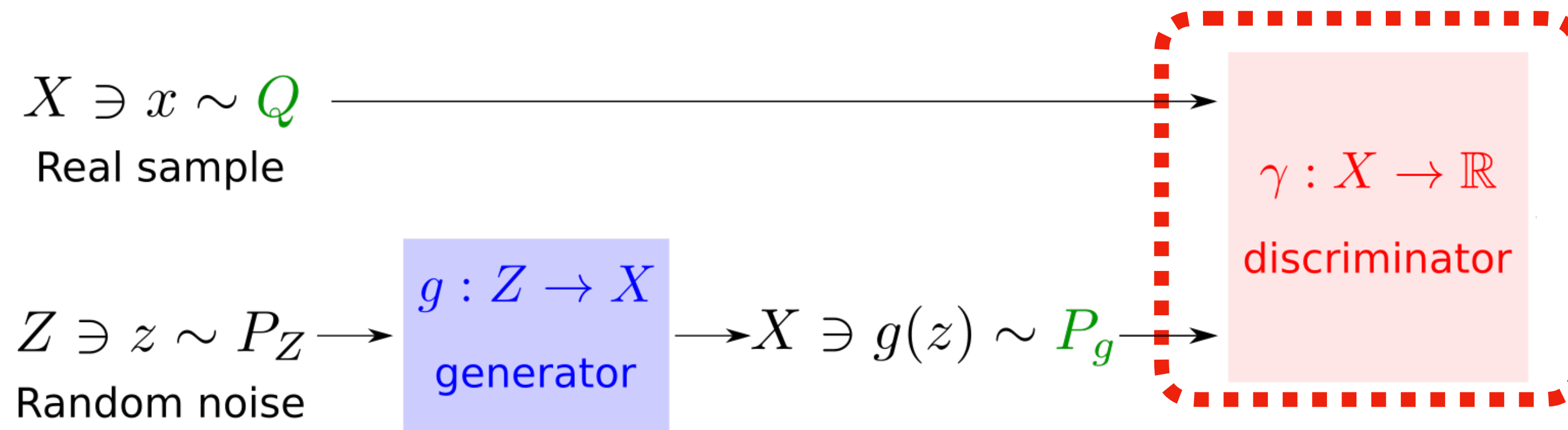
Our Theorem 1: “smarter” discriminator



Theorem: If the distributions P, Q are Σ -invariant, then

$$D^{\Gamma}(Q||P) = D^{\Gamma_{\Sigma}^{inv}}(Q||P),$$

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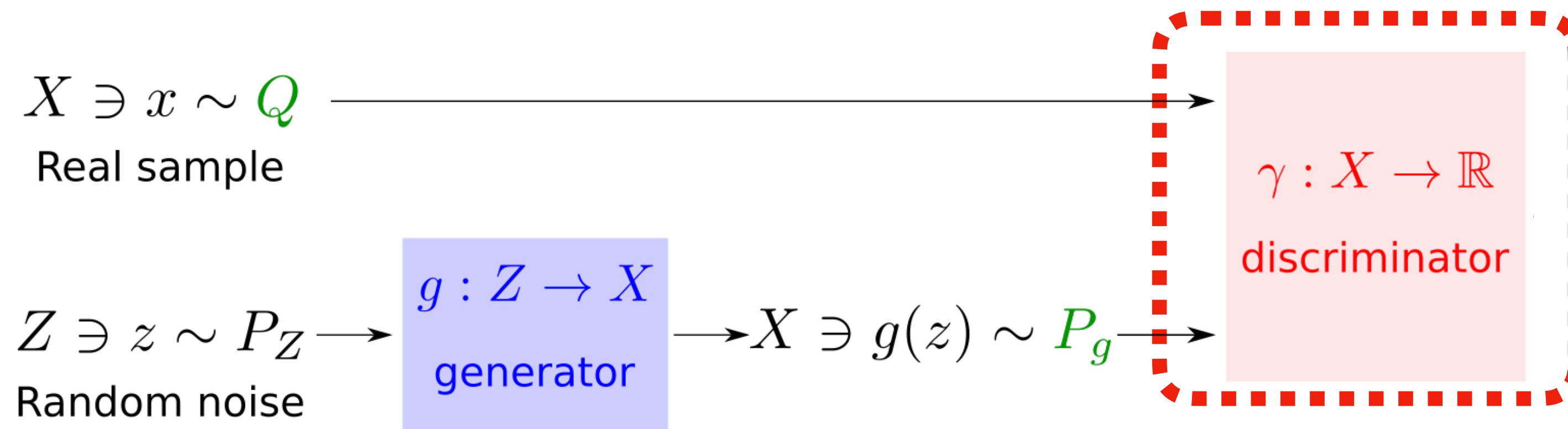


Theorem: If the distributions P, Q are Σ -invariant, then

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- Structure information embedded in the “smarter” space Γ_{Σ}^{inv} of Σ -invariant discriminators

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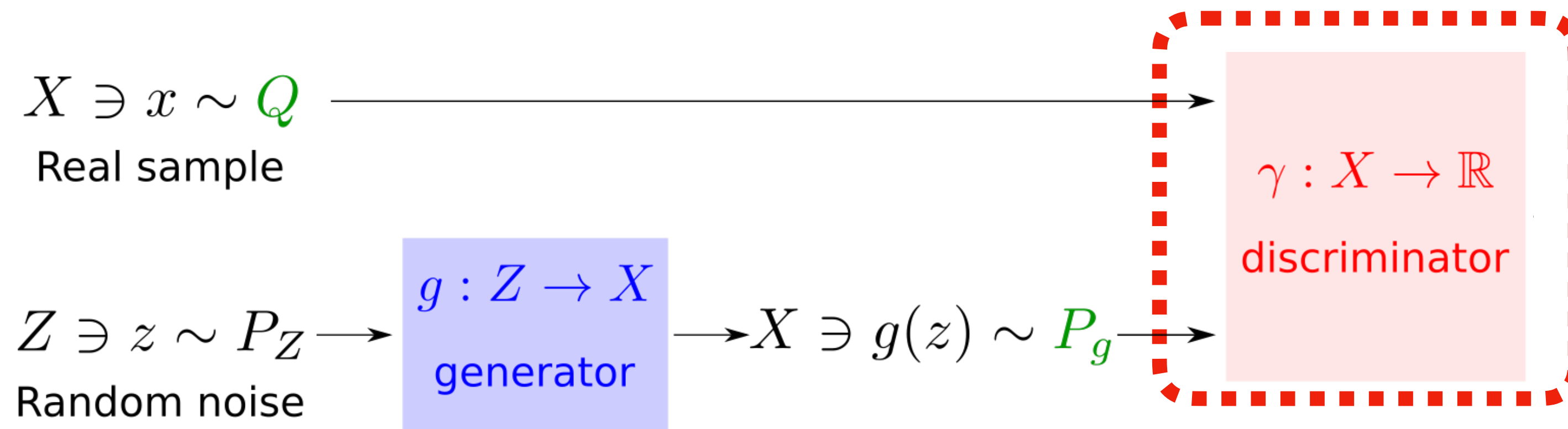


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Our Theorem 1: “smarter” discriminator

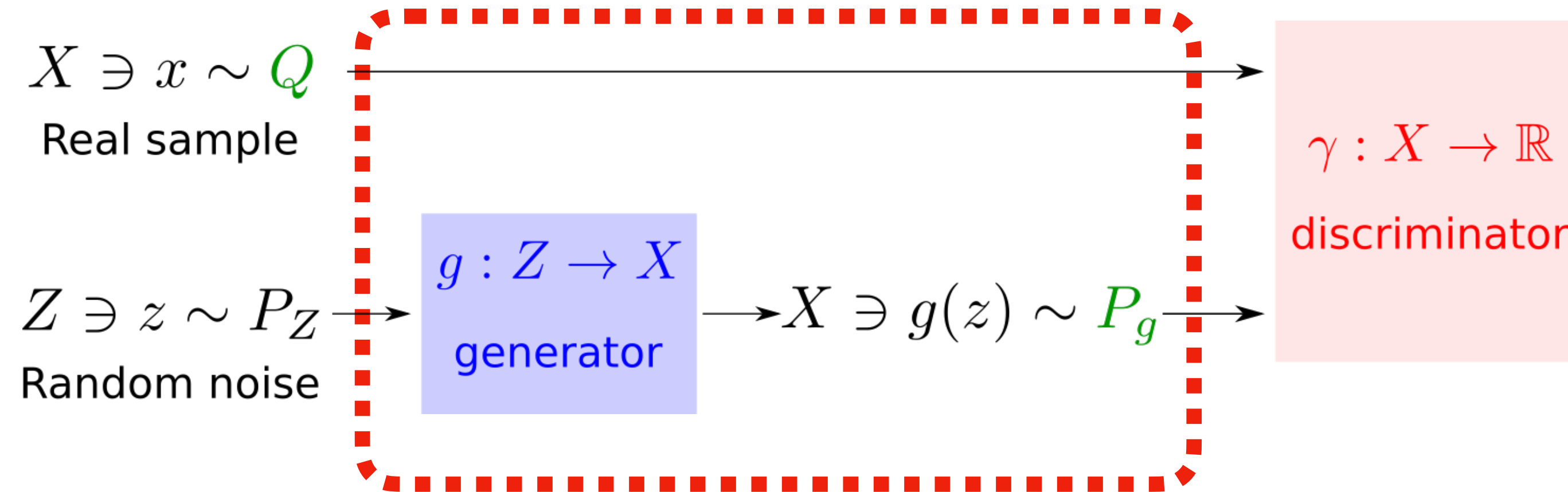


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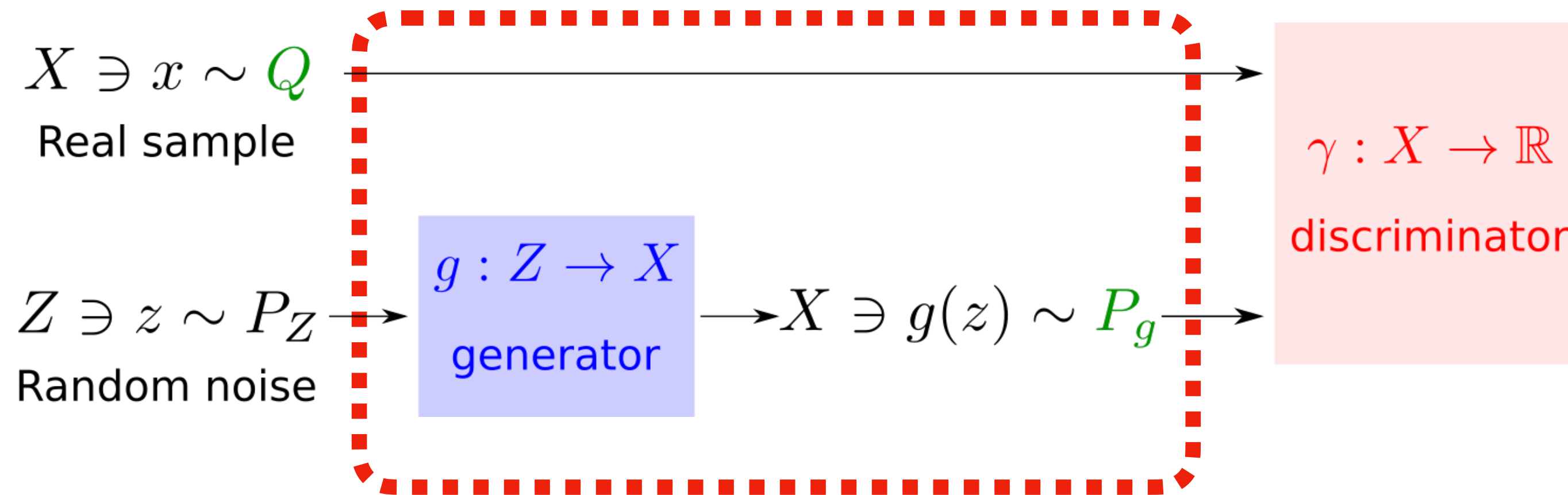
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- Structure information embedded in the “smarter” space Γ_{Σ}^{inv} of Σ -invariant discriminators
- Γ_{Σ}^{inv} is much “smaller” than $\Gamma \implies$ efficient GAN optimization
- Γ_{Σ}^{inv} serves as an unbiased regularization to prevent discriminator overfitting.

Our Theorem 2: “smarter” generator

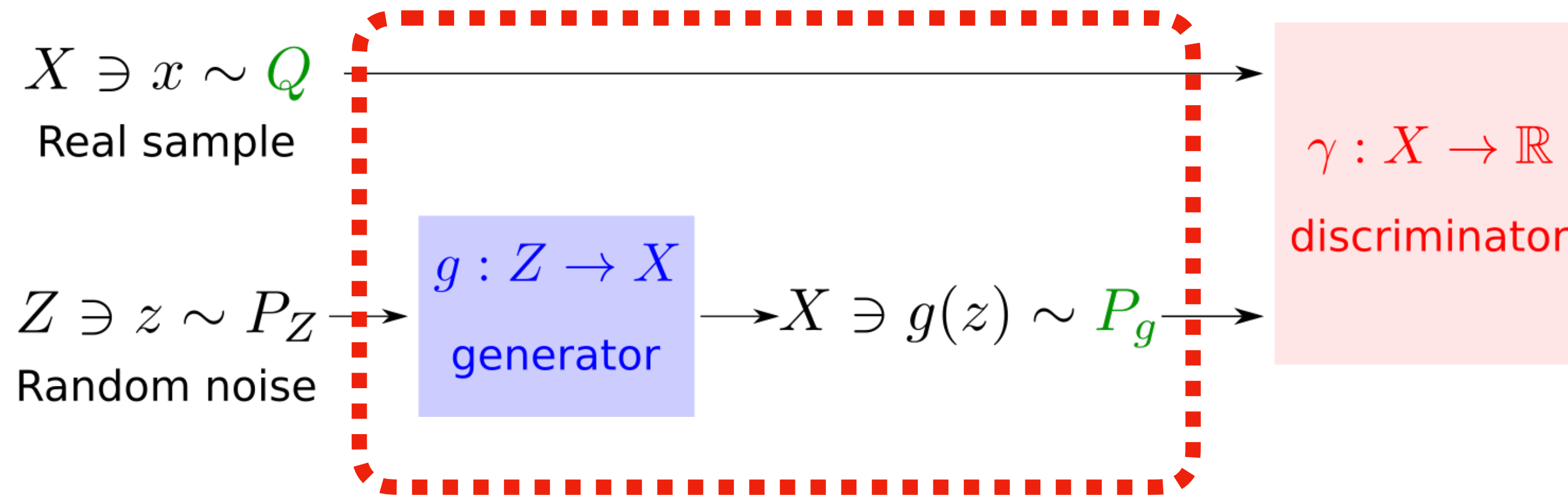


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Theorem: If P_Z is Σ -invariant and $g : Z \rightarrow X$ is Σ -equivariant, the generated measure P_g is Σ -invariant.

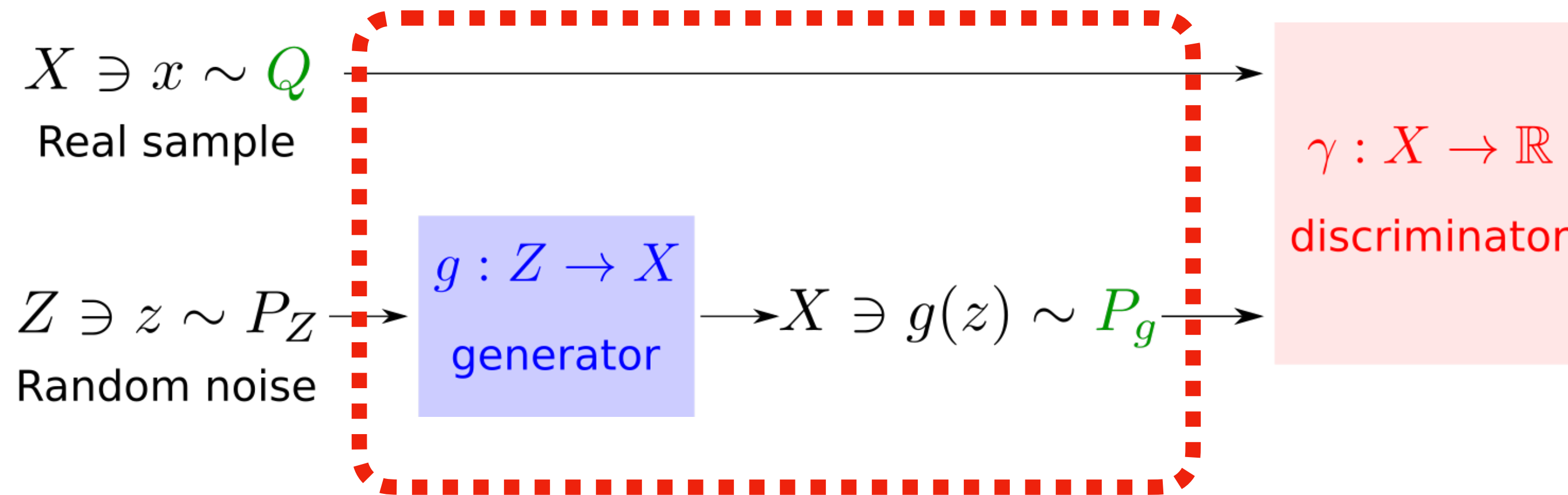
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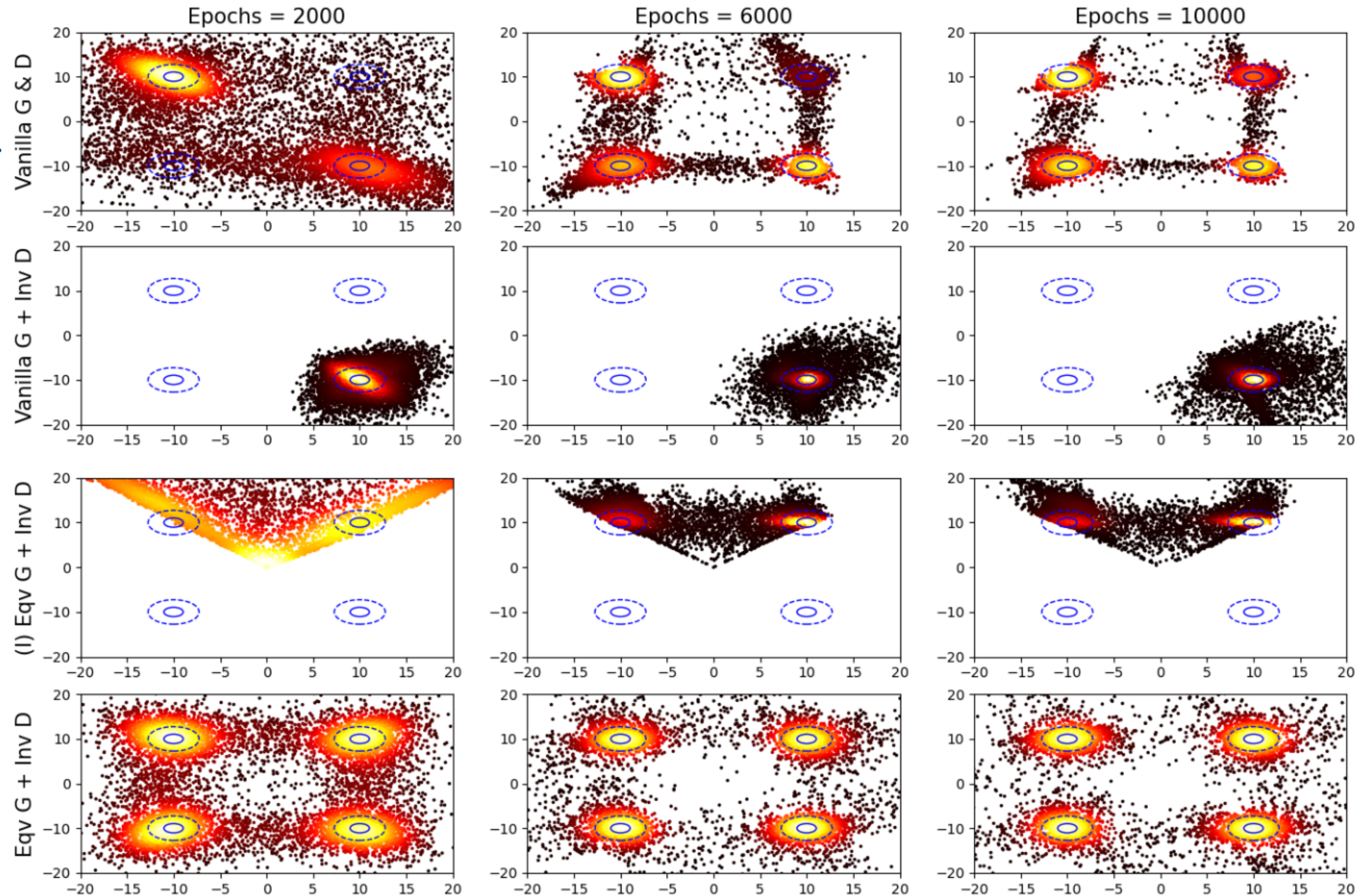


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- Structure information embedded in the "smarter" generator and noise source.
- "Smart" generator and noise source prevents mode collapse.

Two “smart” players

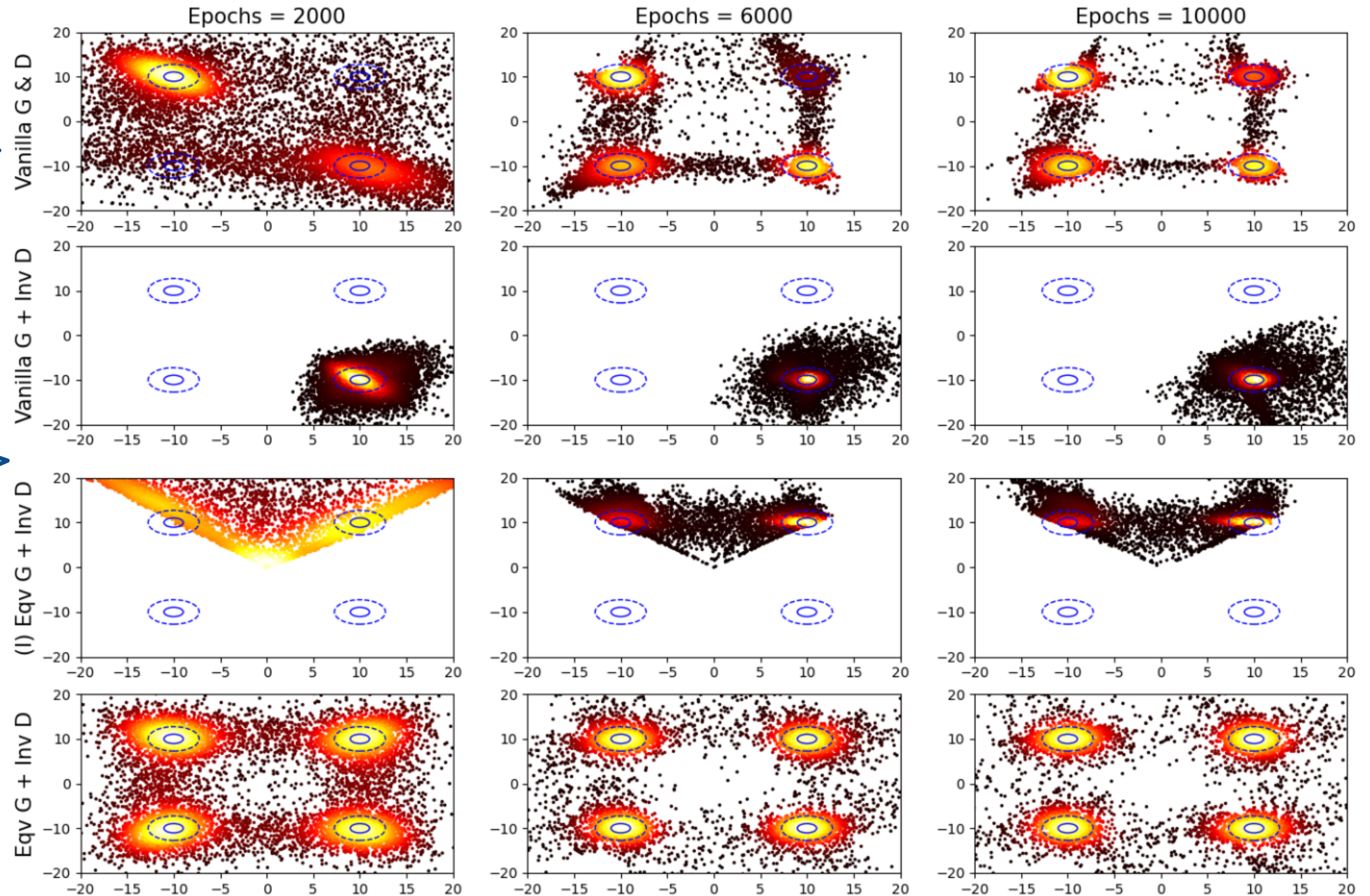
“Ignorant”
players need lots of
data, lots of time...
(the usual GANs)



Two “smart” players

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Players need to be
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weak links!

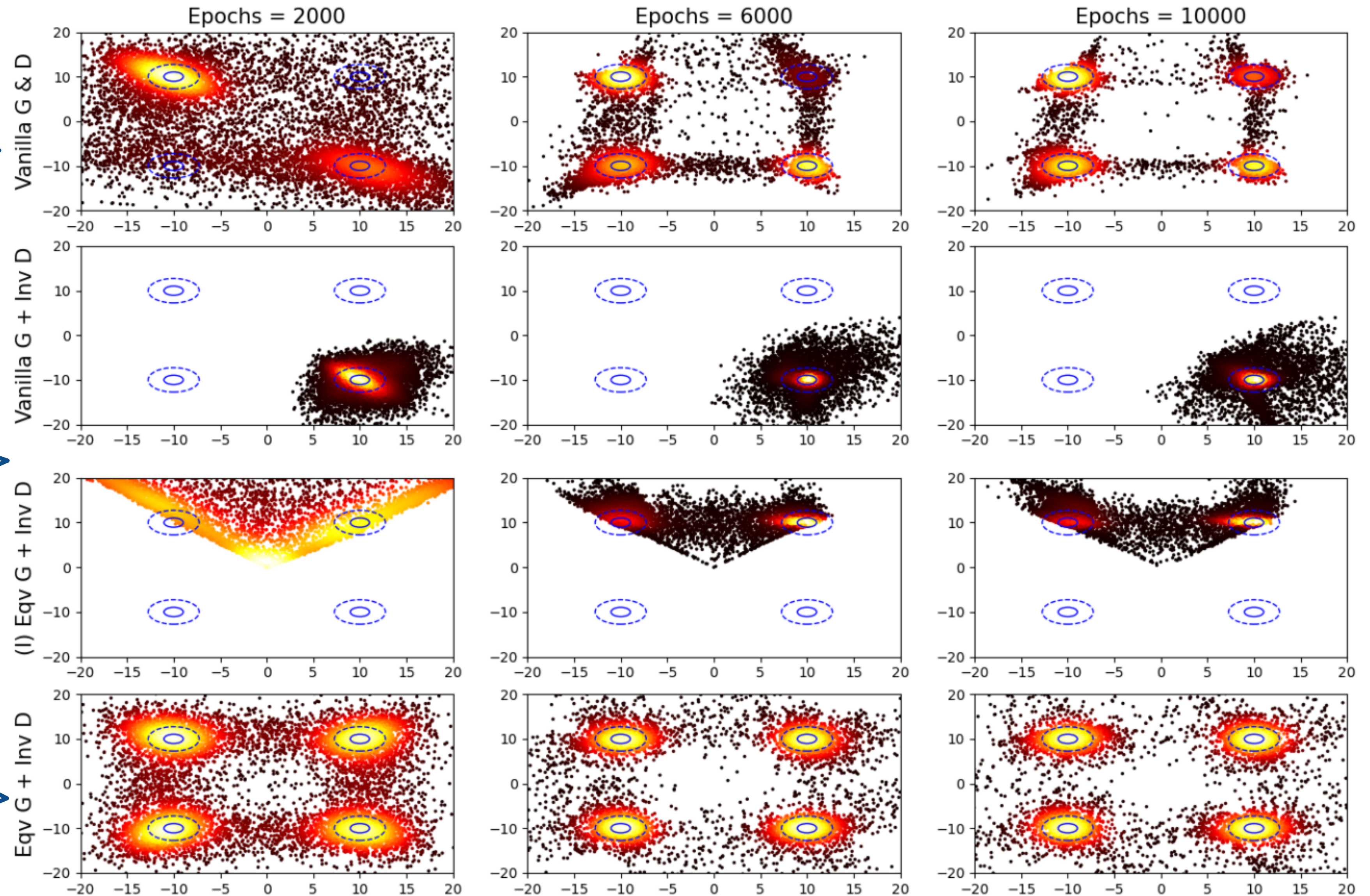


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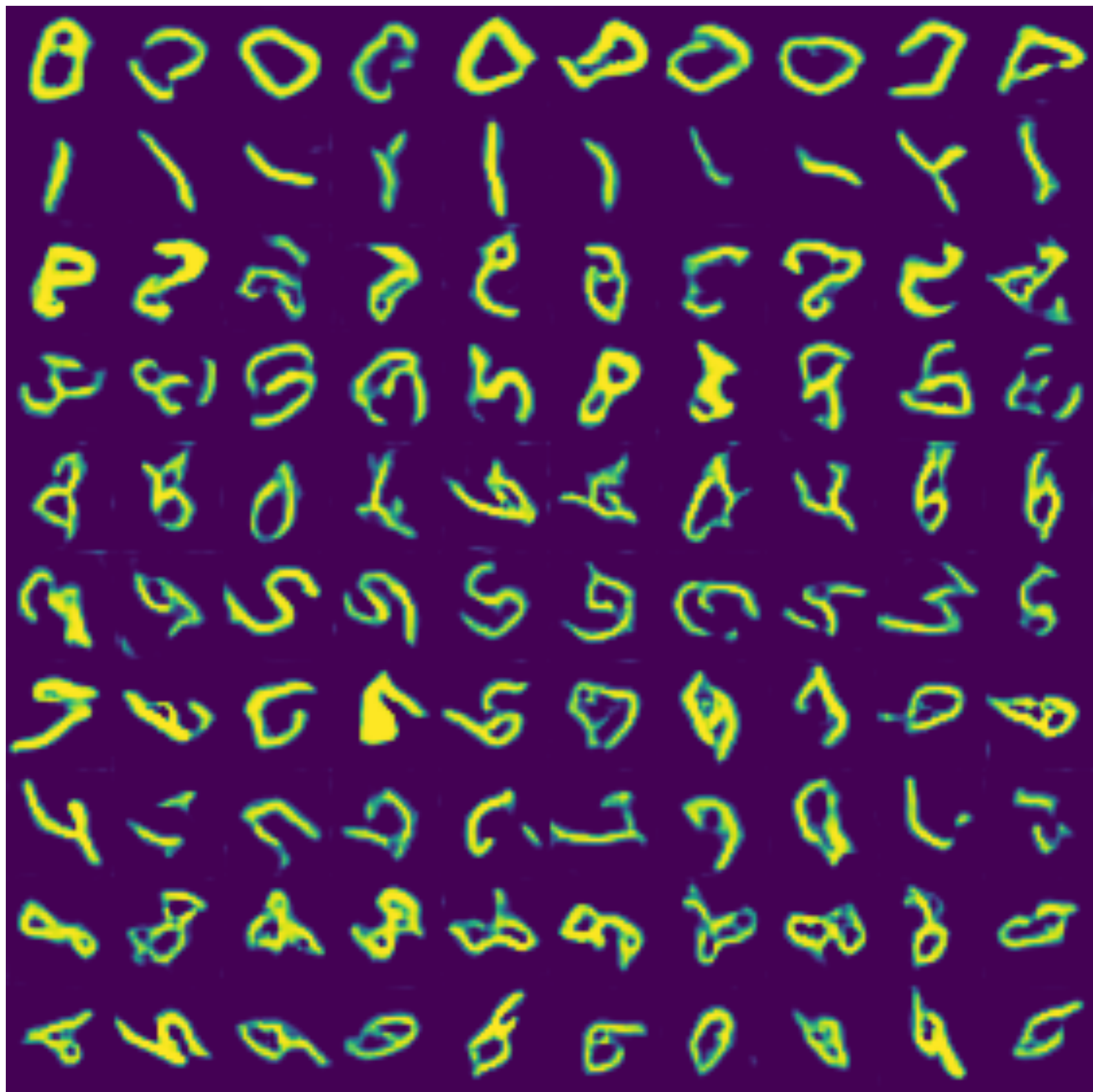
Players need to be
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“Smart” players
learn faster and better
(our GANs)

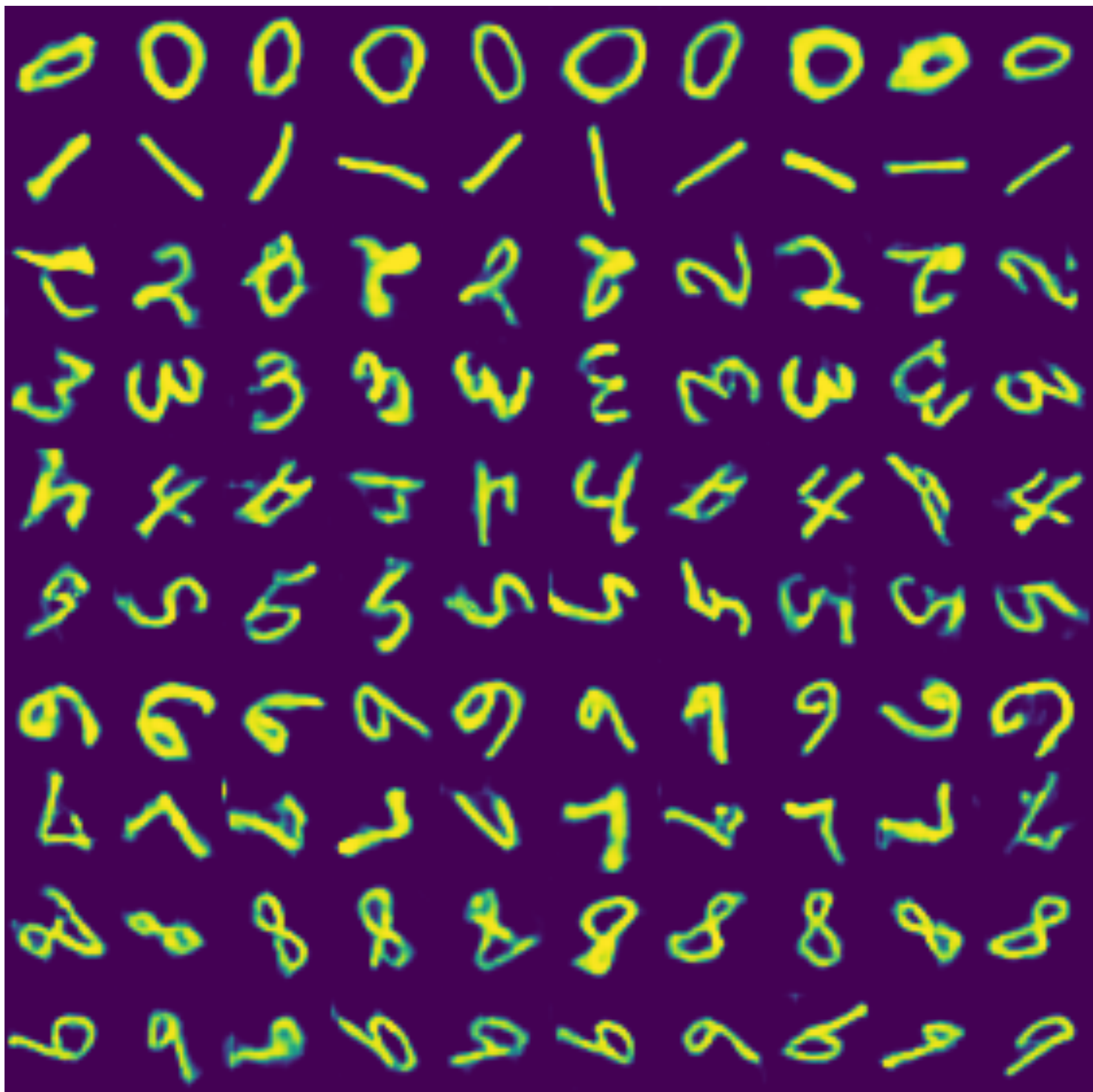


RotMNIST with 1% training samples

“Ignorant” players



“Smart” players



Performance metrics on RotMNIST (FID)

Loss	Architecture	5%	10%	50%	100%
RA-GAN	CNN G&D	357	348	403	392
	Eqv G + CNN D, $\Sigma = C_4$	333	355	380	393
	CNN G + Inv D, $\Sigma = C_4$	181	188	177	176
	(I)Eqv G + Inv D, $\Sigma = C_4$	141	132	135	130
	Eqv G + Inv D, $\Sigma = C_4$	78	89	84	82
	Eqv G + Inv D, $\Sigma = C_8$	52	51	52	57
$D_{\alpha=2}^{\Gamma}$ -GAN	CNN G&D	261	283	297	293
	Eqv G + CNN D, $\Sigma = C_4$	271	251	274	275
	CNN G + Inv D, $\Sigma = C_4$	208	192	183	173
	(I)Eqv G + Inv D, $\Sigma = C_4$	147	133	124	126
	Eqv G + Inv D, $\Sigma = C_4$	99	88	80	81
	Eqv G + Inv D, $\Sigma = C_8$	55	57	53	51

Almost an order of
magnitude
improvement.

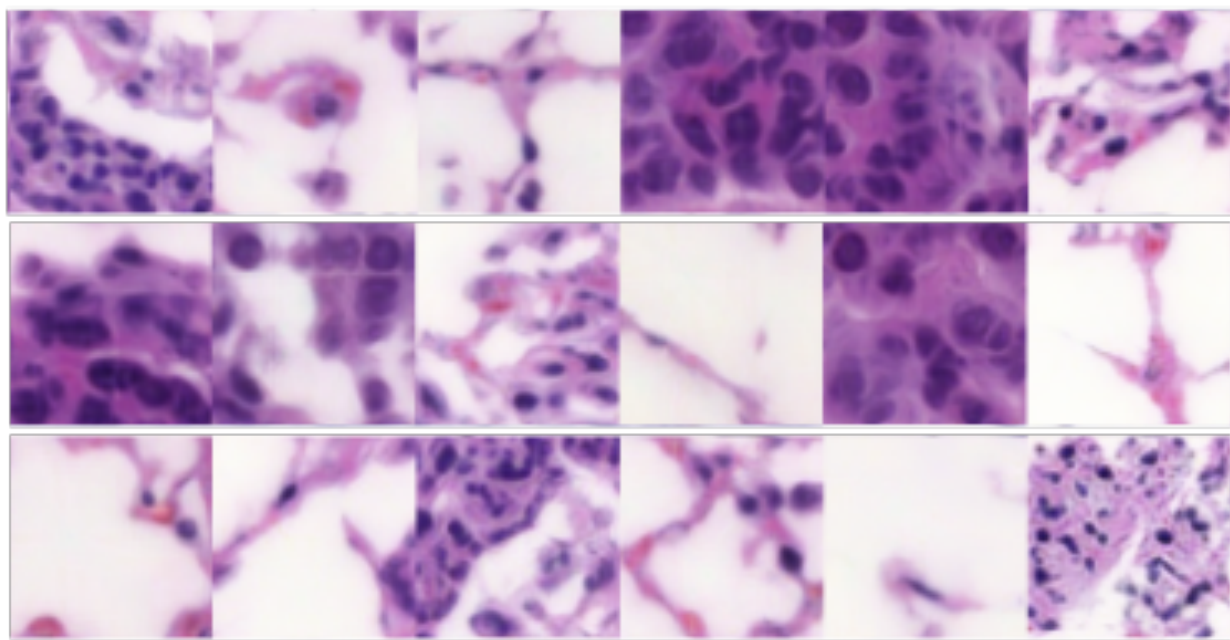
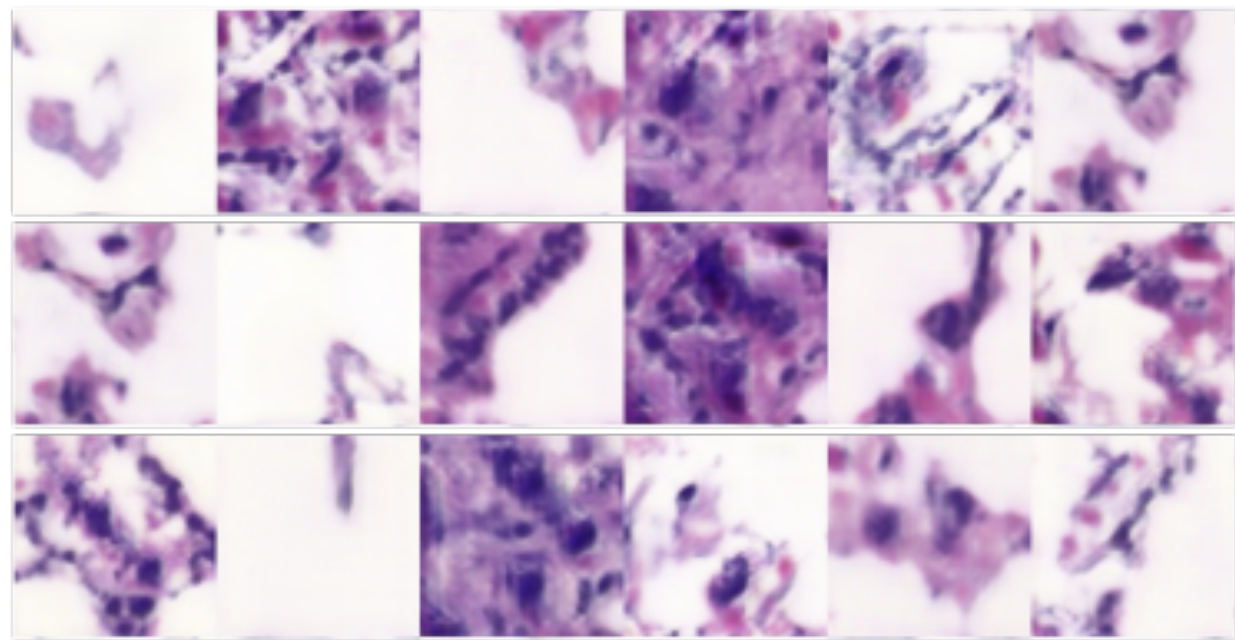
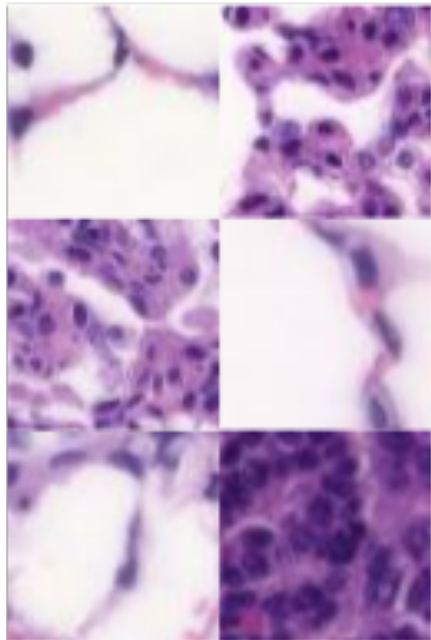
Medical images (ANHIR)

Real Samples

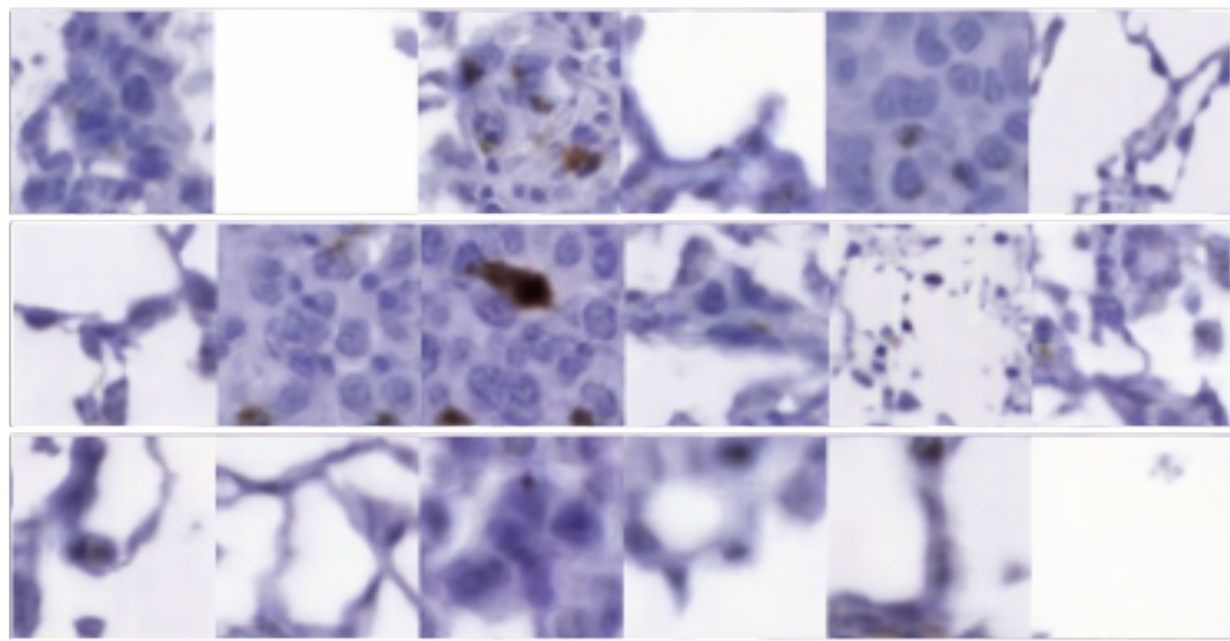
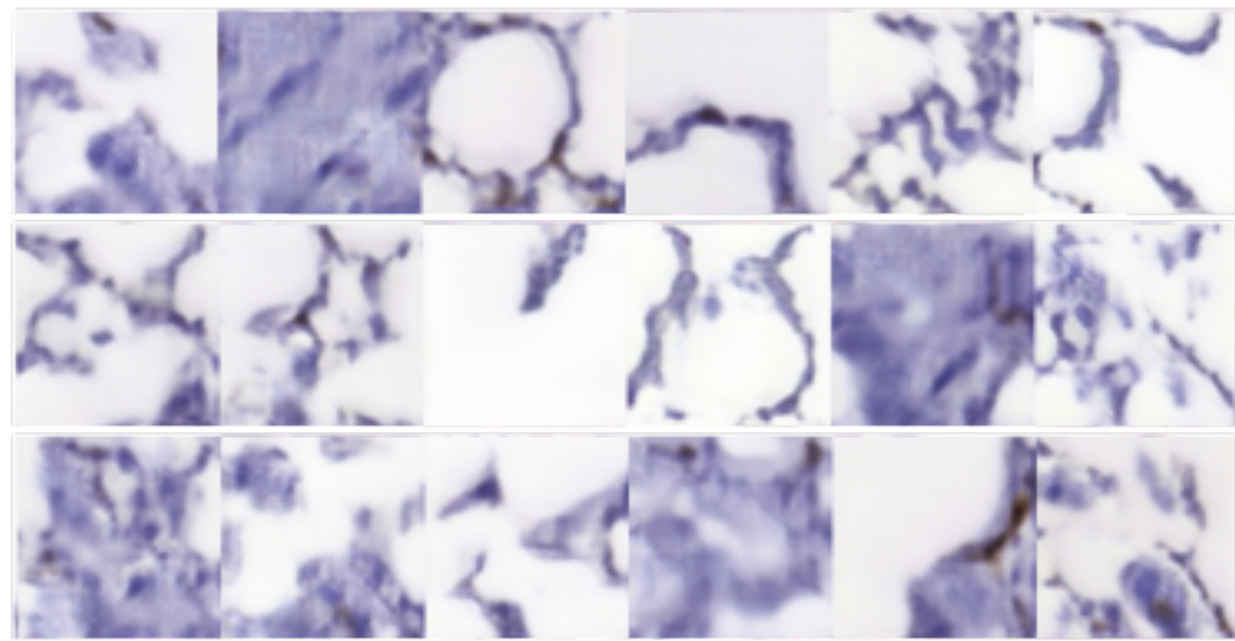
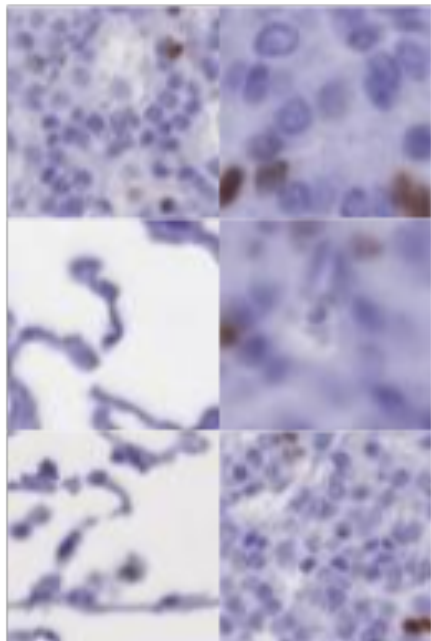
“Ignorant”
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“Smart” players

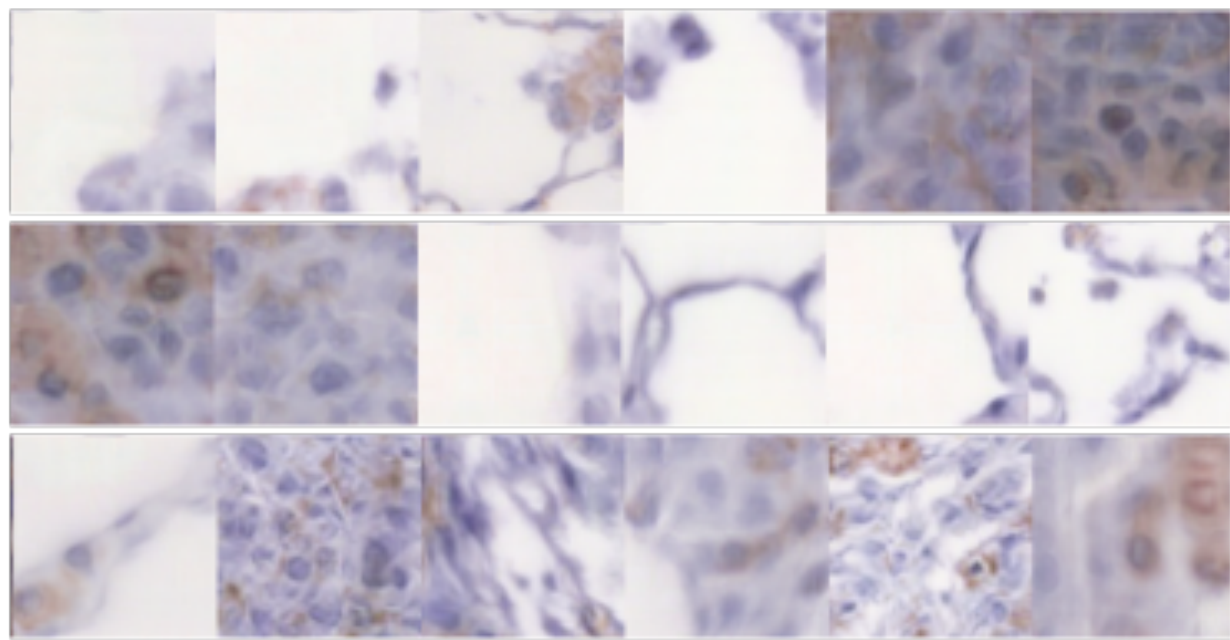
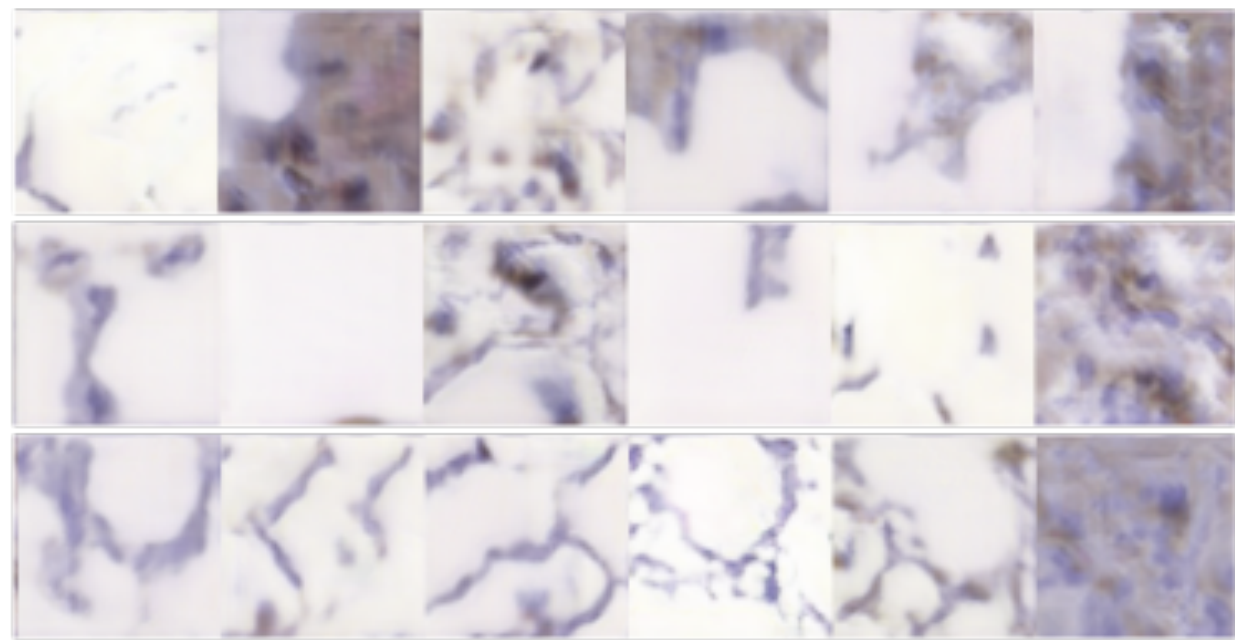
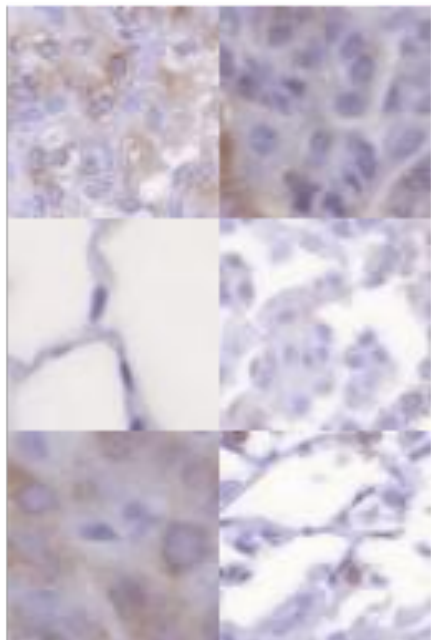
H&E



Ki67



proSPC



Medical images FID (ANHIR)

Loss	Architecture	ANHIR	ANHIR+
RA	CNN G&D	(186, 523)	(184, 503)
	(I) Eqv G + Inv D	(100, 142)	(88, 140)
	Eqv G + Inv D	(78, 125)	(84, 118)
D_2^L	CNN G&D	(313, 485)	(347, 539)
	(I) Eqv G + Inv D	(120, 176)	(119, 177)
	Eqv G + Inv D	(97, 157)	(90, 128)
Loss	Architecture	LYSTO	LYSTO+
RA	CNN G&D	(281, 340)	(250, 312)
	(I) Eqv G + Inv D	(218, 272)	(212, 271)
	Eqv G + Inv D	(175, 238)	(181, 227)
D_2^L	CNN G&D	(289, 410)	(265, 376)
	(I) Eqv G + Inv D	(253, 343)	(244, 329)
	Eqv G + Inv D	(205, 259)	(192, 259)