Physics-constrained GAN for amplitude extraction

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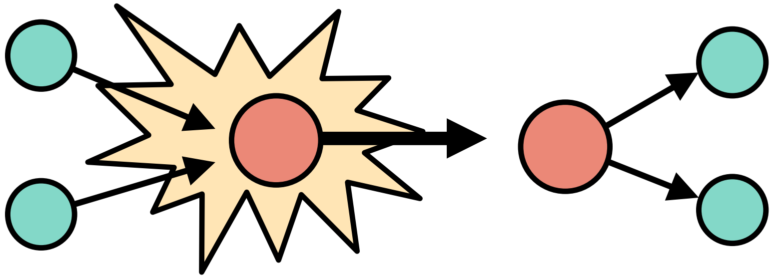
Jefferson Lab JSA A SURA Company A(i)DAPT AI for Data Analysis and PreservaTion JPAC EXOHAD Exotic Hadrons Topical Collaboration

MOTIVATION



The **scattering amplitude** $\mathcal{A}$ is the fundamental quantity of interest in hadron reactions:

- Encodes the underlying dynamics of the interaction
- Crucial for understanding resonance production, decays…
- Is a complex quantity: magnitude + phase

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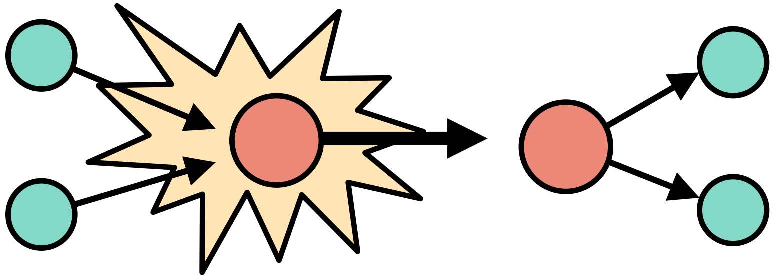

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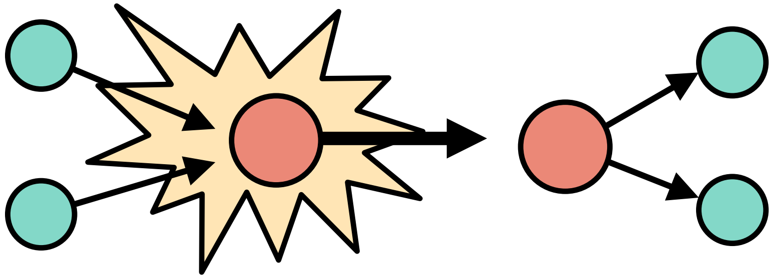
The **cross section** σ is an experimentally observable quantity:

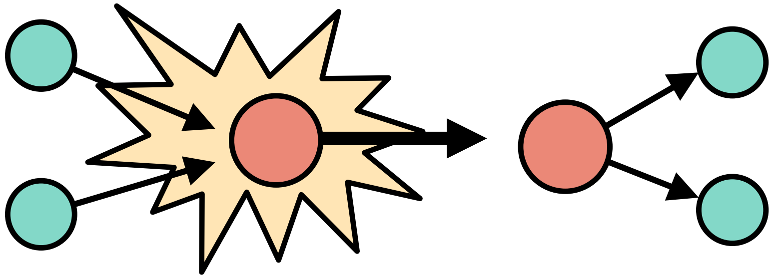
- Related to $|\mathcal{A}|^2$
- The information about the phase is lost

MOTIVATION



The reconstruction of the amplitude from the differential cross section is hard, even for the simplest elastic $2 \to 2$ scattering.

MOTIVATION



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Can we use modern machine-learning techniques to recover the scattering amplitude from experimental data of cross sections?

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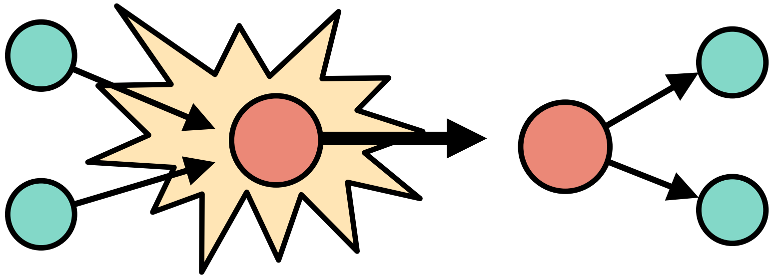

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Why physics-constrained **GANs**?

- Learn distributions and patterns of the (pseudo) data
- Incorporate physics constraints

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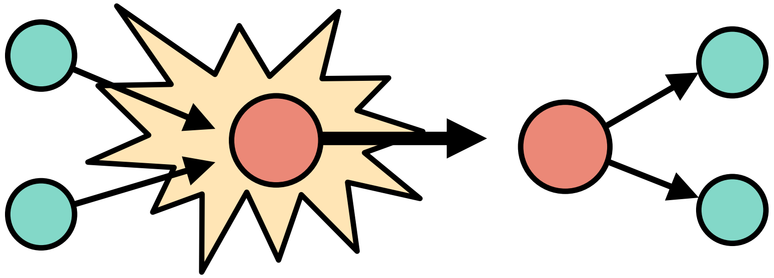

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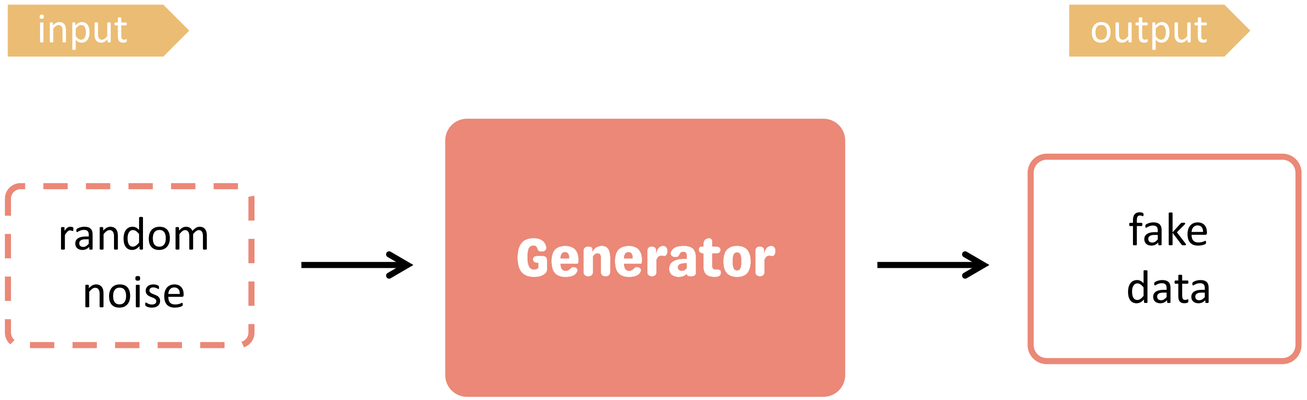
The modulus and phase of the scattering amplitude are related by the **unitarity relation**.

INTRODUCTION TO GANs

Two neural networks:

- The **generator** needs to capture the data distribution

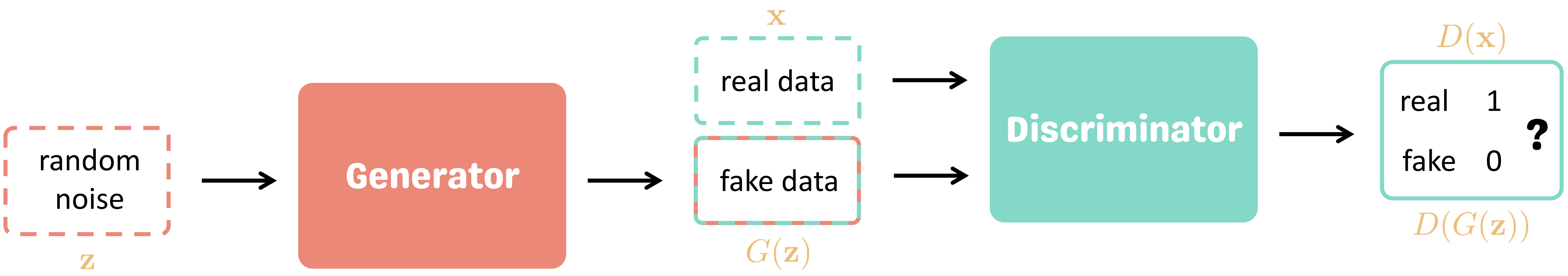


INTRODUCTION TO GANs

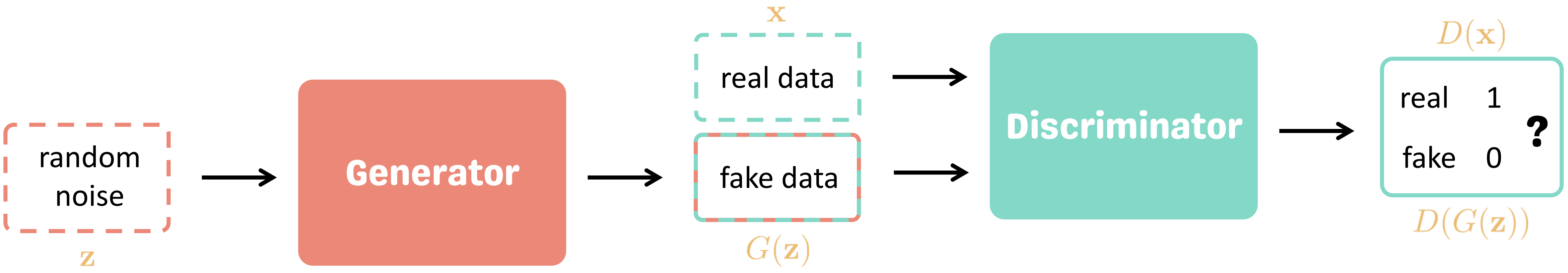
Two neural networks:

- The **generator** needs to capture the data distribution
- The **discriminator** estimates the probability that a sample comes from the training data rather than from the generator

INTRODUCTION TO GANs



INTRODUCTION TO GANs

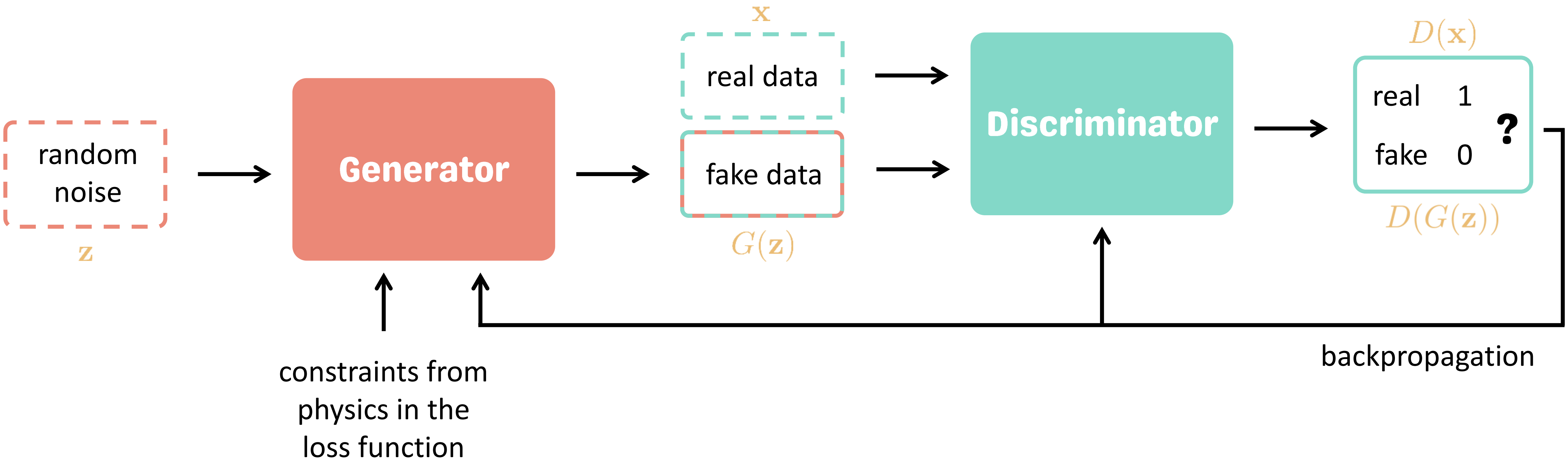


GAN Minmax Game

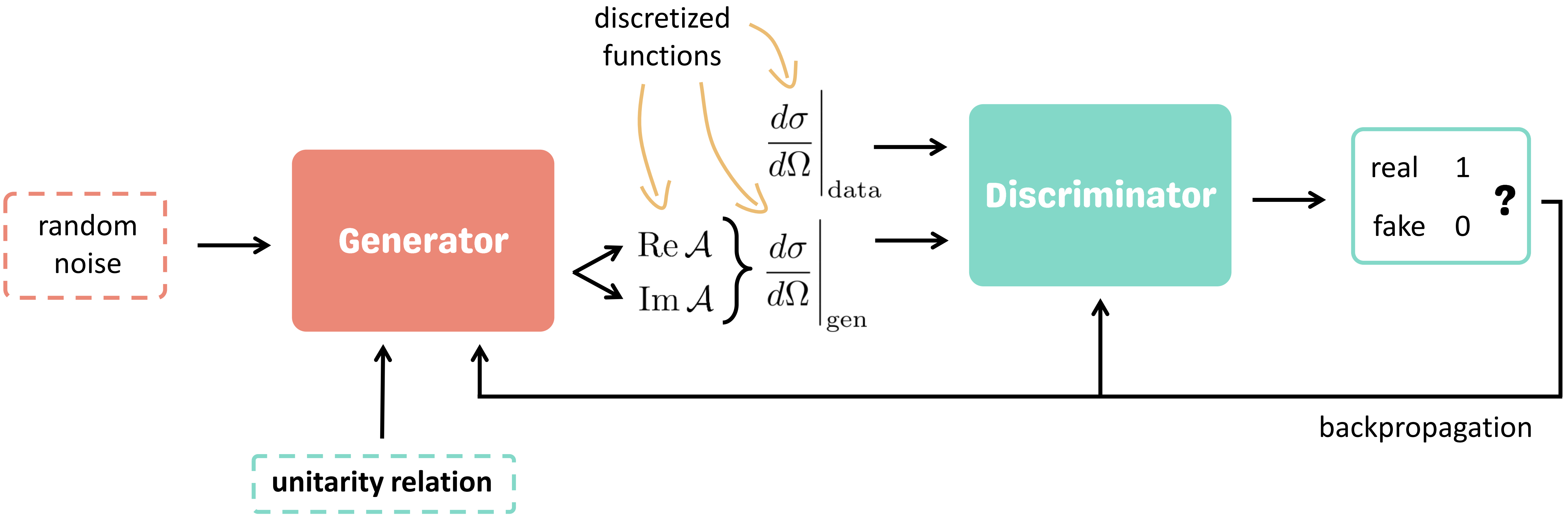
$$\min_G \max_D V(D,G) = \underbrace{\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}(\mathbf{x})}[\log D(\mathbf{x})]}_{\text{real data}} + \underbrace{\mathbb{E}_{\mathbf{z}\sim p_z(\mathbf{z})}[\log(1 - D(G(\mathbf{z})))]}_{\text{fake data}}$$

	real data	fake data
G minimizes ↓	N/A	*D* classifies as 0
D maximizes ↑	*D* classifies as 1	*D* classifies as 0

INTRODUCTION TO GANs



INTRODUCTION TO GANs



PHYSICS PROBLEM

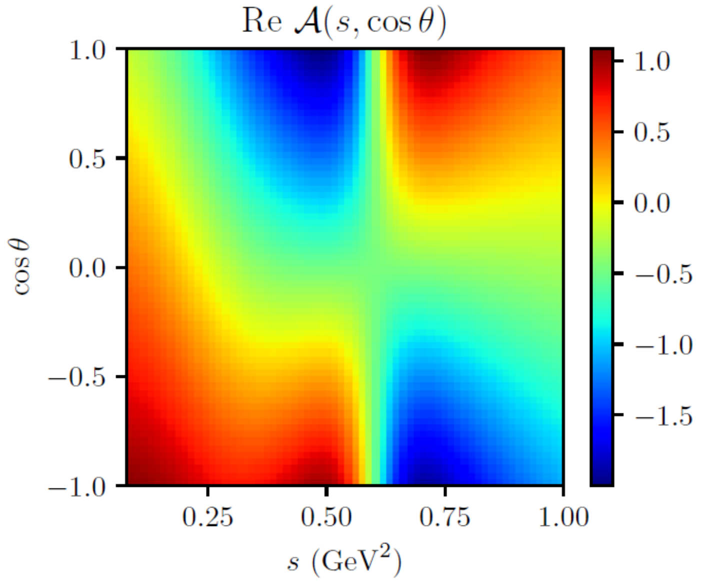
Elastic scattering $\pi^+\pi^- \to \pi^+\pi^-$

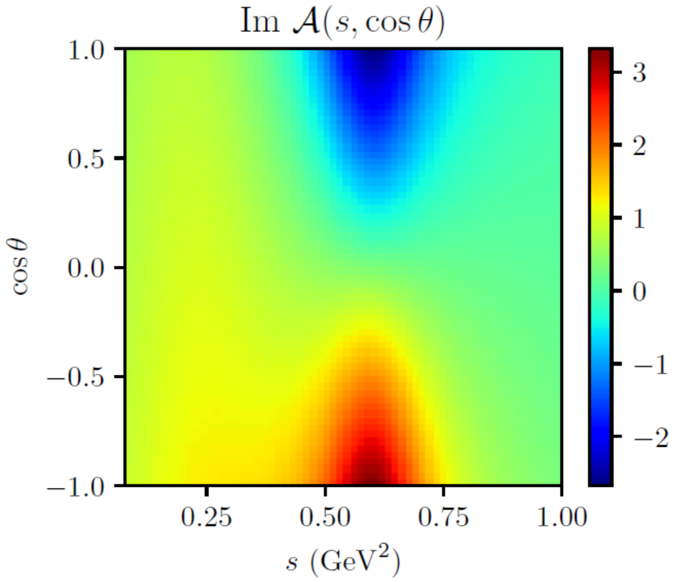
➔ dominated by $f_0(500)$ and $\rho(770)$ resonances

$$\mathcal{A}(s, \cos\theta) = \sum_{\ell=0}^{n} (2\ell+1) f_\ell(s) P_\ell(\cos\theta)$$

Partial-wave decomposition of the amplitude truncated to $n = 1$ and Breit-Wigner type partial waves:

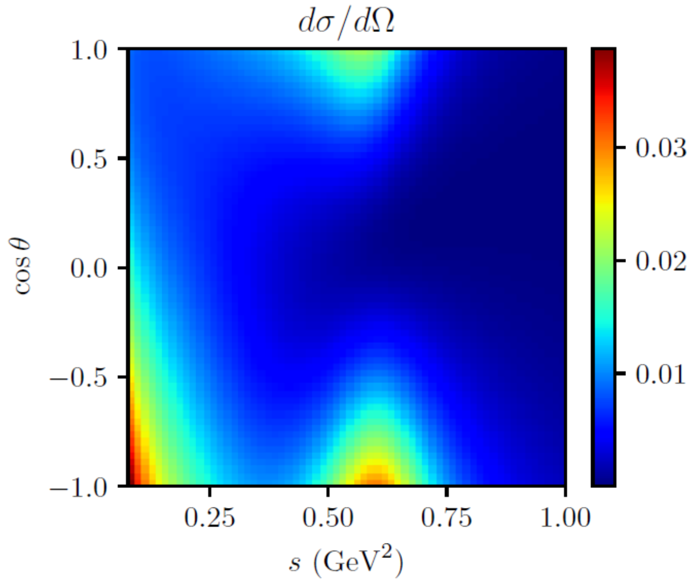
$$\mathcal{A}(s, \cos\theta) = f_0(s) + 3 f_1(s) \cos\theta \qquad f_\ell = \frac{m_\ell \Gamma_\ell}{m_\ell^2 - s - i m_\ell \Gamma_\ell}$$





Differential cross section

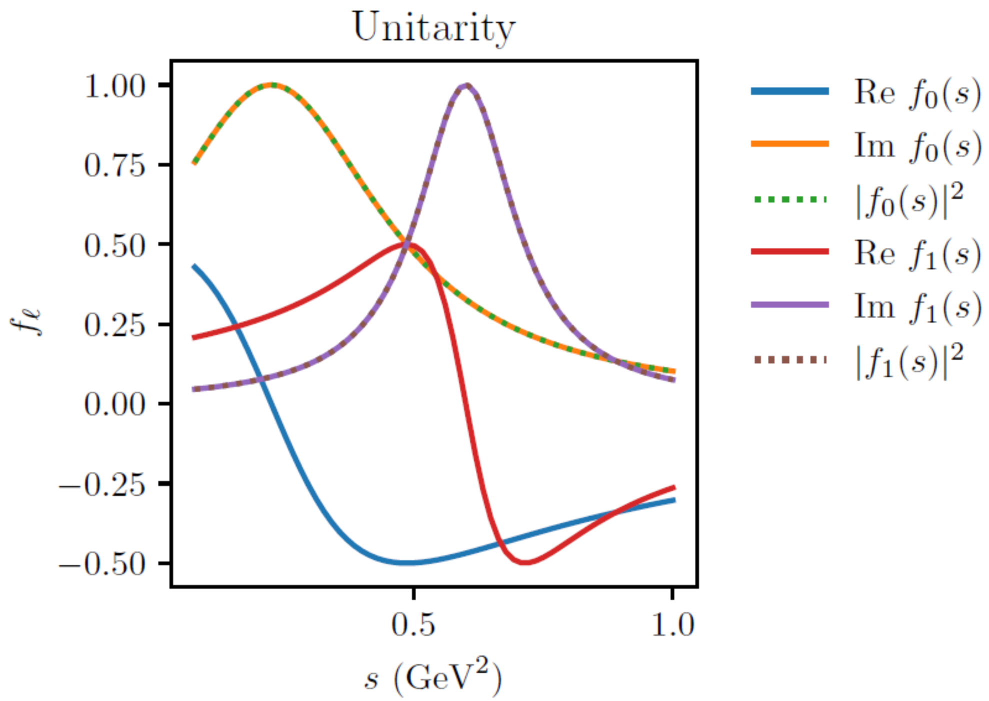
$$\frac{d\sigma}{d\Omega} = \frac{1}{64\pi^2} \frac{1}{s} |\mathcal{A}(s, \cos\theta)|^2$$



PHYSICS PROBLEM

- Unitarity of the partial waves

$$\text{Im } f_\ell(s) = |f_\ell(s)|^2$$



$$f_\ell(s) = \frac{1}{2}\int_{-1}^{+1} dz P_\ell(z)\mathcal{A}(s,z)$$

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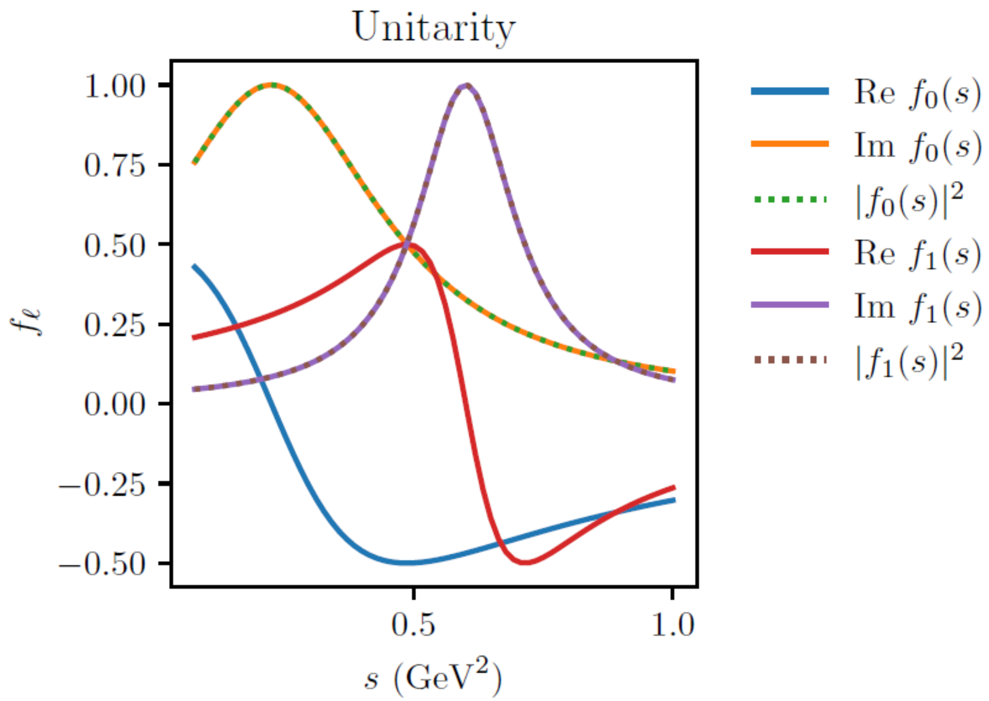

$$f_\ell(s) = \frac{1}{2}\int_{-1}^{+1} dz P_\ell(z)\mathcal{A}(s,z)$$

- Integral unitarity relation for the full amplitude

$$\text{Im } \mathcal{A}(s,z) = \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_{-1}^{+1} dz' \mathcal{A}(s,z')\mathcal{A}^*(s,z'')$$

$$z'' = zz' + \sqrt{1-z^2}\sqrt{1-z'^{\,2}}\cos\phi$$

or, equivalently

$$\sin\Phi(s,z) = \int_0^{2\pi} d\phi \int_{-1}^{+1} dz' \frac{|\mathcal{A}(s,z')||\mathcal{A}(s,z'')|}{4\pi|\mathcal{A}(s,z)|} \times \cos\left[\Phi(s,z') - \Phi(s,z'')\right]$$

Phase ambiguity: $\mathcal{A}(s,z) \to -\mathcal{A}^*(s,z)$

$$\Phi(s,z) \to \pi - \Phi(s,z)$$

IMPLEMENTATION DETAILS

python
PyTorch

GAN architecture:

Generator

Layer Type	Input Dimensions	Output Dimensions	Activation/Other Details
Fully Connected	(batch_size, noise_dim)	(batch_size, $4 \times 4 \times 1024$)	BatchNorm, LeakyReLU (0.2)
Reshape	(batch_size, $4 \times 4 \times 1024$)	(batch_size, 4, 64, 64)	Reshapes tensor
ConvTranspose2d (1)	(batch_size, 4, 64, 64)	(batch_size, 64, 64, 64)	BatchNorm, LeakyReLU (0.2), Kernel=17
ConvTranspose2d (2)	(batch_size, 64, 64, 64)	(batch_size, 64, 64, 64)	BatchNorm, LeakyReLU (0.2), Kernel=17
ConvTranspose2d (3)	(batch_size, 64, 64, 64)	(batch_size, 64, 64, 64)	BatchNorm, LeakyReLU (0.2), Kernel=17
ConvTranspose2d (4)	(batch_size, 64, 64, 64)	(batch_size, 64, 64, 64)	BatchNorm, LeakyReLU (0.2), Kernel=17
Conv2d (Final)	(batch_size, 64, 64, 64)	(batch_size, 2, 64, 64)	Produces 2-channel image output

Lambda

Layer Type	Input Dimensions	Output Dimensions	Transformation Details
Lambda	(batch_size, 2, 64, 64)	(batch_size, 1, 64, 64)	Maps generator output to discriminator input

Discriminator

Layer Type	Input Dimensions	Output Dimensions	Activation/Other Details
Conv2d (1)	(batch_size, 1, 64, 64)	(batch_size, 64, 32, 32)	LeakyReLU (0.2), Dropout (0.3), Kernel=4
Conv2d (2)	(batch_size, 64, 32, 32)	(batch_size, 128, 16, 16)	BatchNorm, LeakyReLU (0.2), Dropout (0.3)
Flatten	(batch_size, 128, 16, 16)	(batch_size, $128 \times 16 \times 16$)	Flattens for FC layers
Fully Connected (1)	(batch_size, $128 \times 16 \times 16$)	(batch_size, 64)	LeakyReLU (0.2), Dropout (0.3)
Fully Connected (2)	(batch_size, 64)	(batch_size, 1)	Outputs real/fake score

IMPLEMENTATION DETAILS

python
PyTorch

GAN architecture:

Generator

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Too complex?
Too simple?

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IMPLEMENTATION DETAILS

- Loss Functions:

MSE Loss Measure the mean squared error between the target and output.

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(\mathrm{output}_i - \mathrm{target}_i)^2$$

Unitarity Loss Enforce unitarity by comparing the modulus squared of the integral of the scattering amplitudes over angular variables to the imaginary part.

$$\mathcal{L}_\mathrm{u} = \frac{1}{N \cdot N_s \cdot N_z}\sum_{i=1}^{N}\sum_{j=1}^{N_s}\sum_{k=1}^{N_z}\left(\left|\mathrm{Im}\,\mathcal{A}(s,z) - \mathrm{Re}\,\mathcal{I}(s,z)\right| + \left|\mathrm{Im}\,\mathcal{I}(s,z)\right|\right)$$

with $\mathcal{I}(s,z) = \frac{1}{4\pi}\int_{-1}^{1} dz' \int_{0}^{2\pi} d\phi \left(\mathcal{A}(s,z')\mathcal{A}(s,z''(z,z',\phi))\right)$

Integral approximator: Simpson's rule

Integral sampling points: $[\cos\theta \times \phi] = 64 \times 10$

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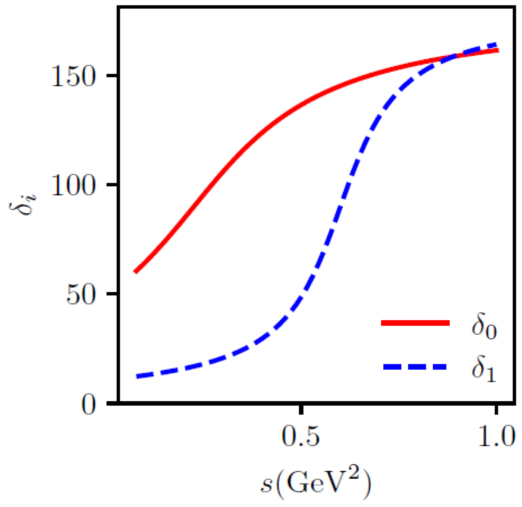
d0 Loss Ensure the positive derivative of the f_0 phase shift.

d1 Loss Ensure the positive derivative of the f_1 phase shift.

$$\delta_\ell = \mathrm{atan}\left(\frac{\mathrm{Im}\,f_\ell(s)}{\mathrm{Re}\,f_\ell(s)}\right)$$

$$\mathcal{L}_{D_\ell} = \frac{1}{N}\sum_{i=1}^{N}\log\big(\max\big(0, -\Delta\delta_\ell(s)\big)+1\big), \qquad f_\ell(s) = \frac{1}{2}\int_{-1}^{+1} dz P_\ell(z)\mathcal{A}(s,z)$$



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with $\mathcal{I}(s,z) = \frac{1}{4\pi}\int_{-1}^{1}dz'\int_{0}^{2\pi}d\phi\left(\mathcal{A}(s,z')\mathcal{A}(s,z''(z,z',\phi)\right)\right)$

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Better way to constrain the phase?

d0 Loss Ensure the positive derivative of the f_0 phase shift.

d1 Loss Ensure the positive derivative of the f_1 phase shift.

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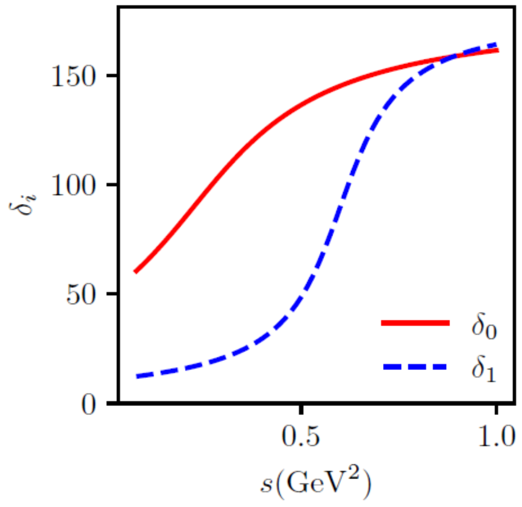

$$\mathcal{L}_{D_\ell} = \frac{1}{N}\sum_{i=1}^{N}\log\left(\max\left(0, -\Delta\delta_\ell(s)\right) + 1\right), \qquad f_\ell(s) = \frac{1}{2}\int_{-1}^{+1}dz P_\ell(z)\mathcal{A}(s,z)$$

IMPLEMENTATION DETAILS

- Other hyperparameters:

Generator Optimizer	Adam Learning rate: 0.0001
Discriminator Optimizer	Adam Learning rate: 0.00001
Batch Size	256
Training Size	40×256
Input Noise Dimension	100
Epochs	Total: 200 (with stopping if convergence achieved)
Weights for Generator Losses	[MSE, unitarity, d0, d1] = [1,1,10,10]
Device	GPU

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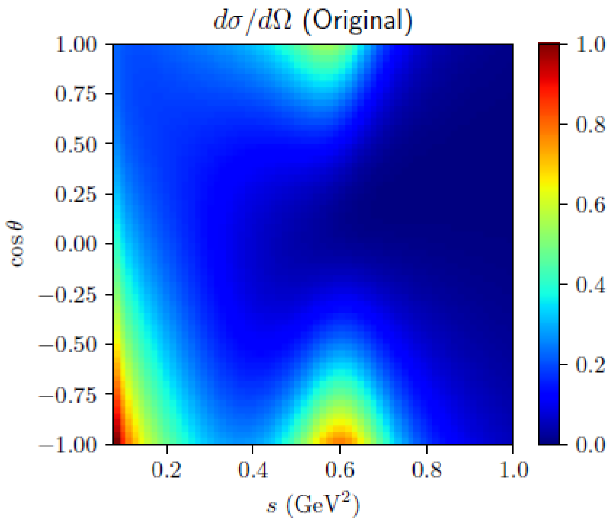
How to optimize?

TRAINING DATASET

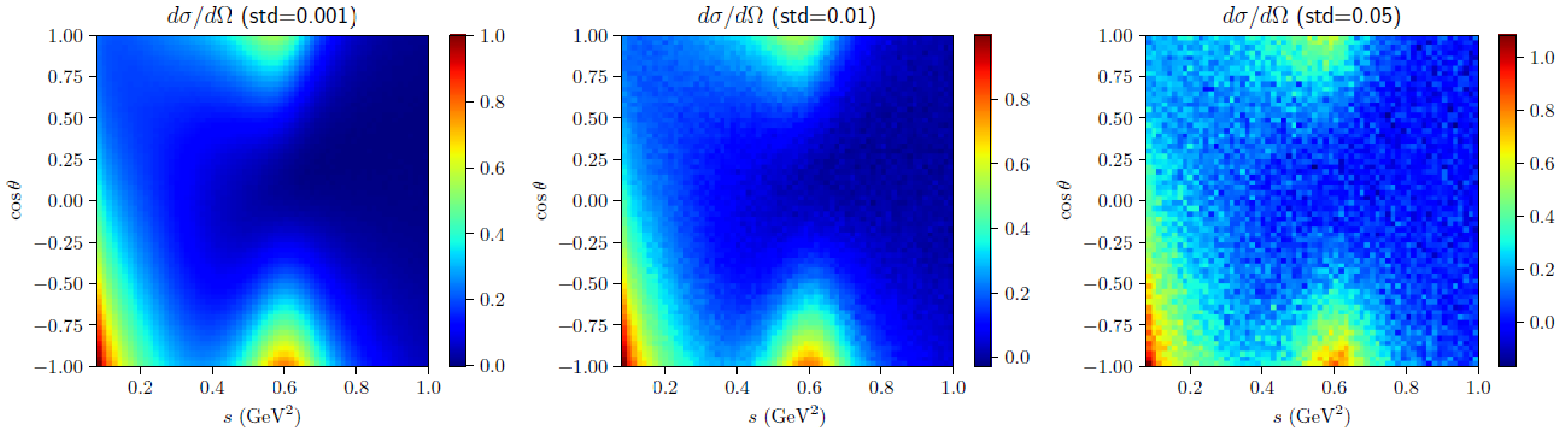


Normalized differential cross section discretized in grid:

$$64 \times 64,\ \ s \in [(2m_\pi)^2, 1\ \text{GeV}^2],\ \ \cos\theta \in [-1, 1]$$

Training samples with additional gaussian noise:

$$40 \times \text{BATCH\_SIZE} = 40 \times 256\ \ \text{samples}$$



PRELIMINARY RESULTS

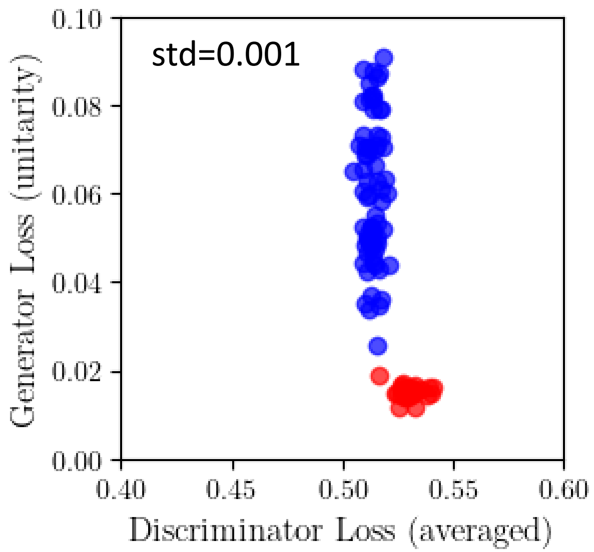
- Trained 100 GANs for 200 epochs:

Stop training if unitarity loss is smaller than 0.02 and changes less than 0.01 and for 10 consecutive epochs:

$$\mathcal{L}_{\mathrm{u}} < 0.02$$

$$\mathcal{L}_{\mathrm{u},n} - \mathcal{L}_{\mathrm{u},n-1} < 0.01$$

29/100 converged



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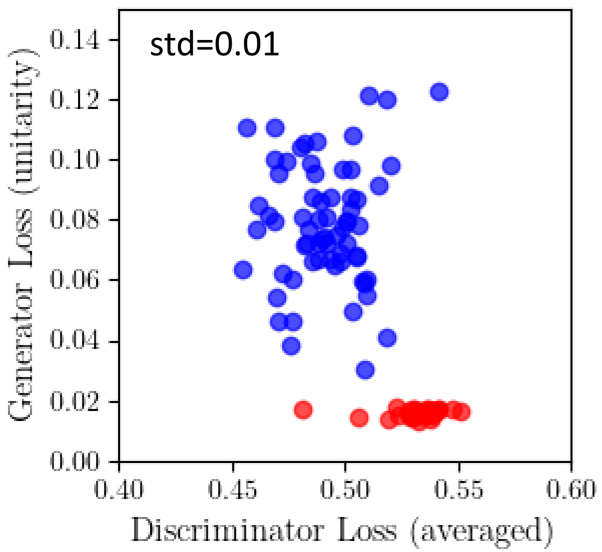
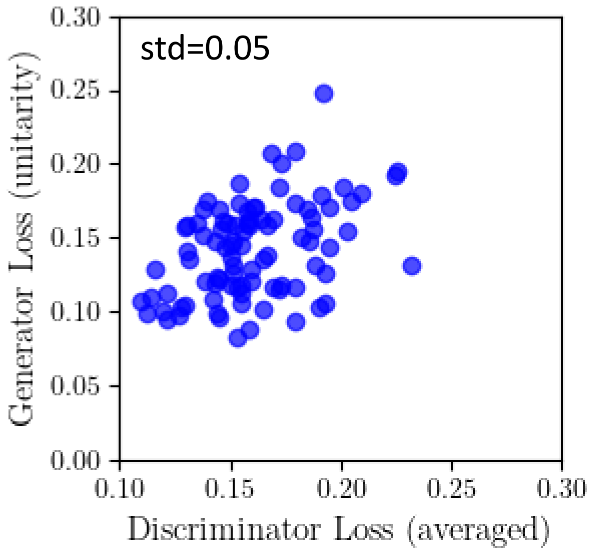
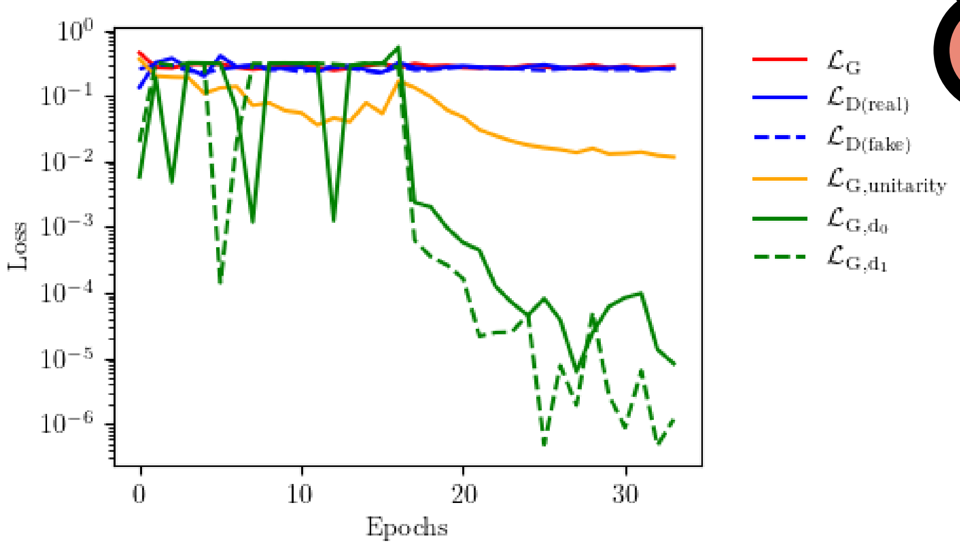


0/100 converged

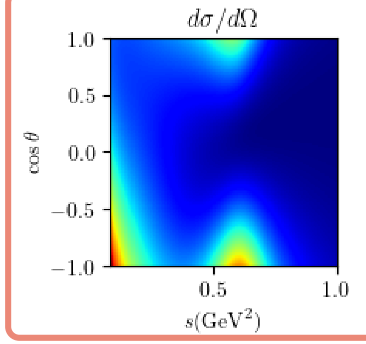


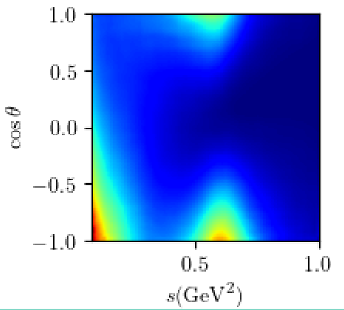
PRELIMINARY RESULTS

- Example of converged GAN with std=0.01:



model ("true" without noise)





generated ("fake")

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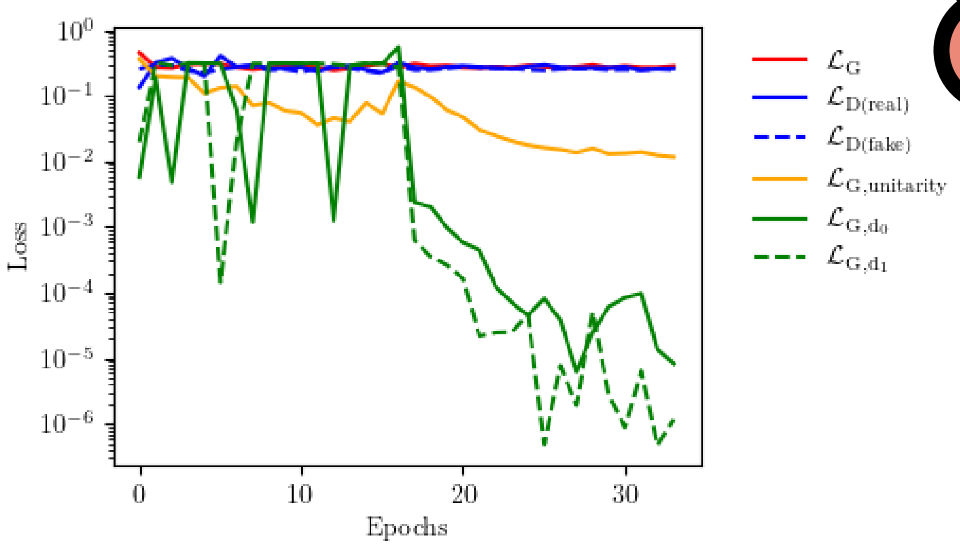

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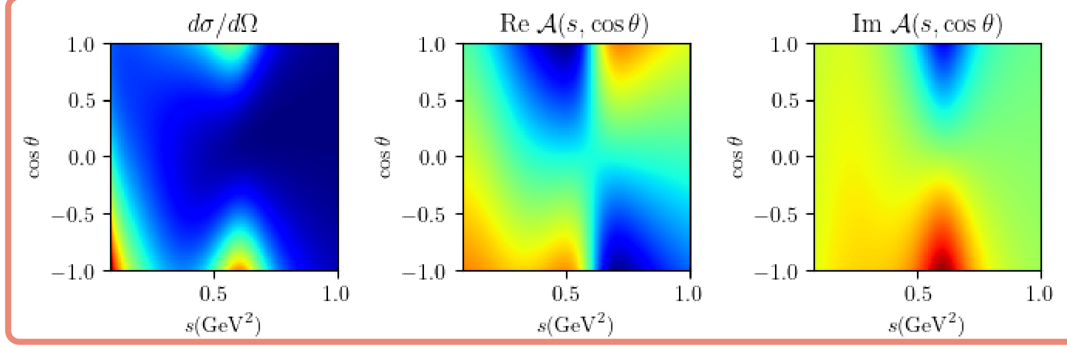

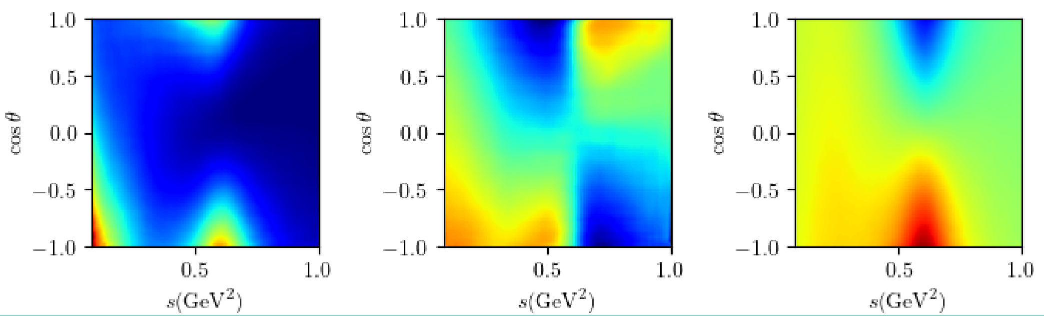

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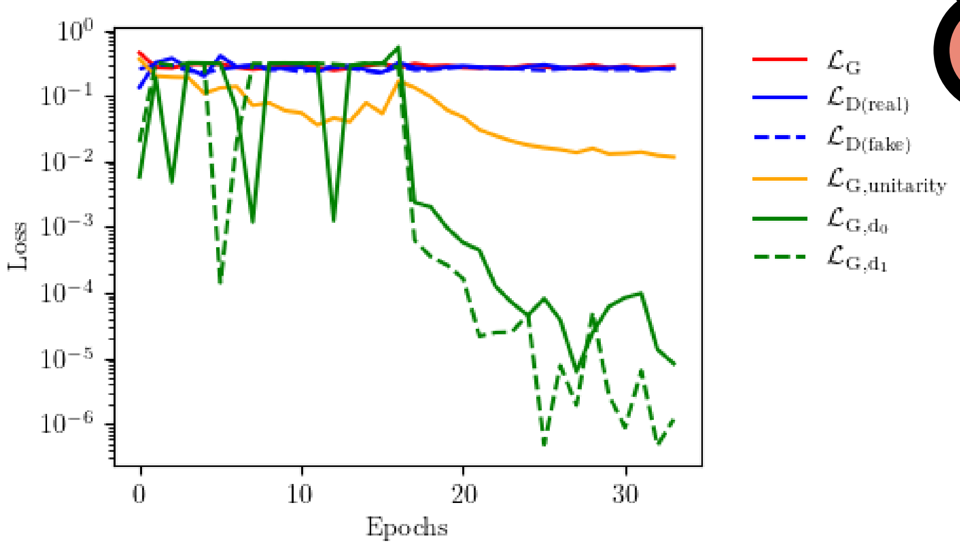

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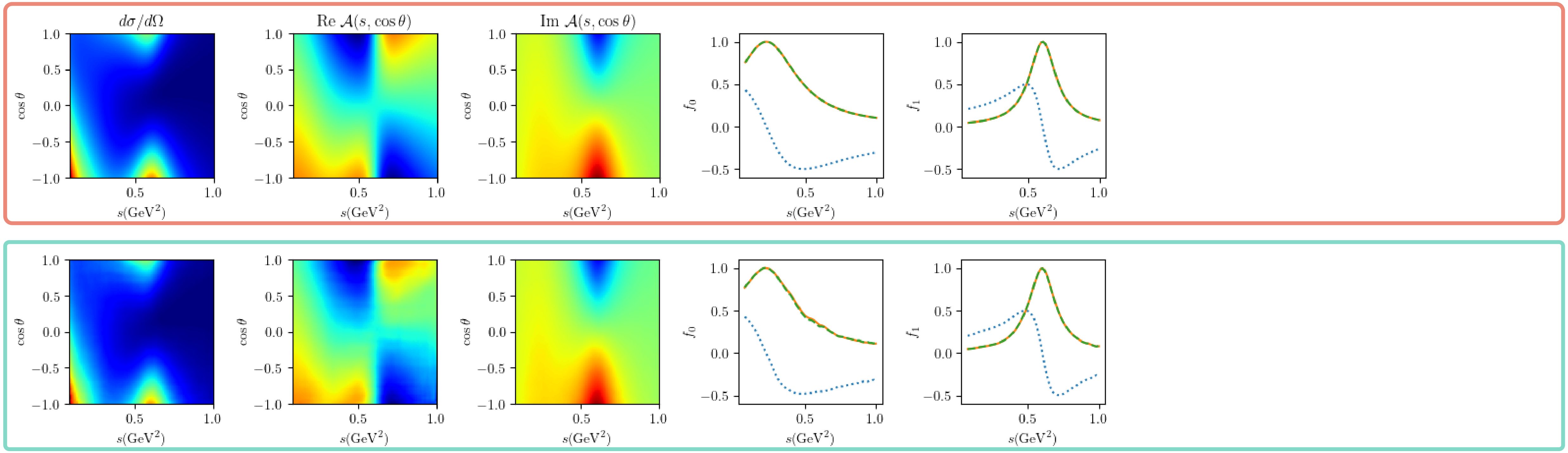

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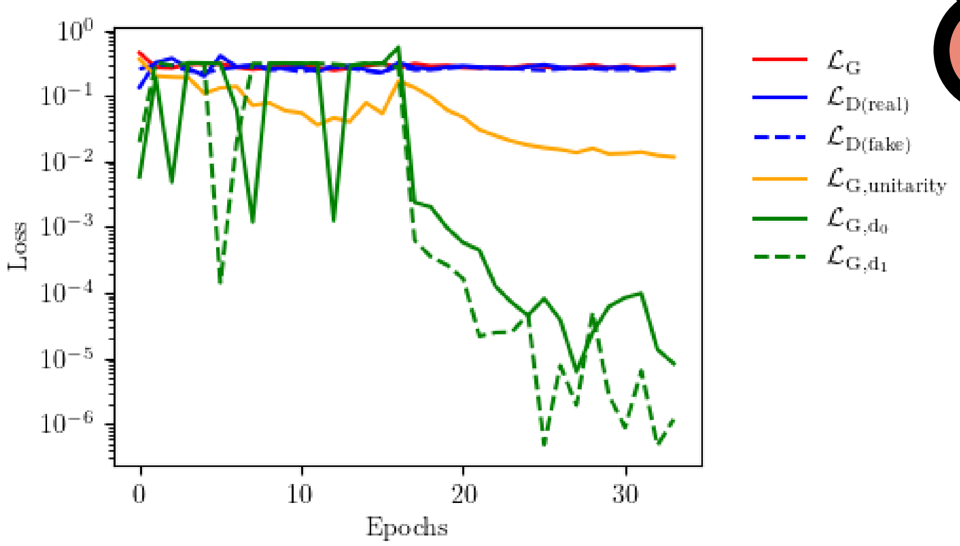
PRELIMINARY RESULTS



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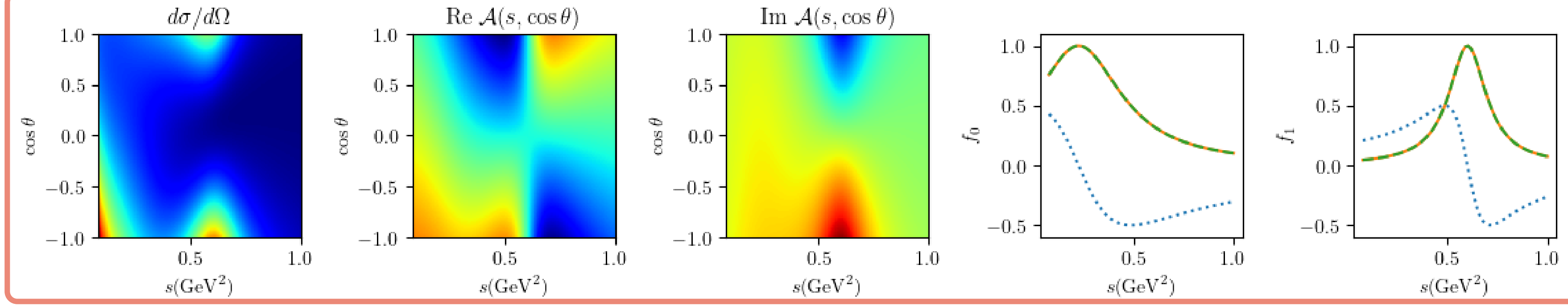
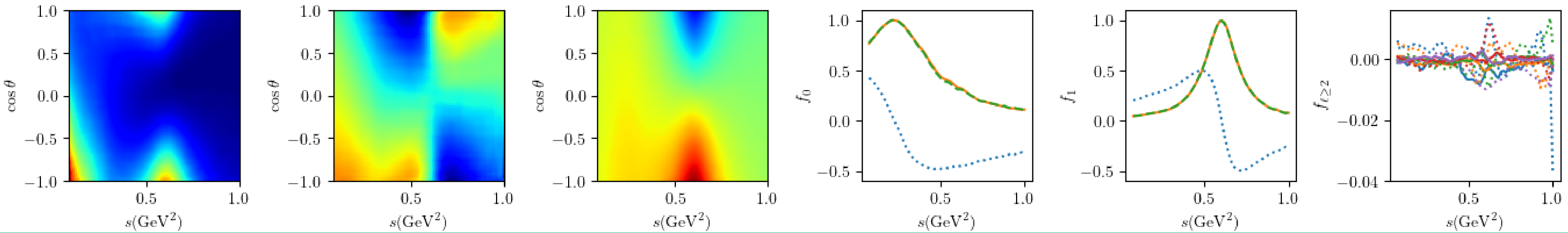
model ("true" without noise)

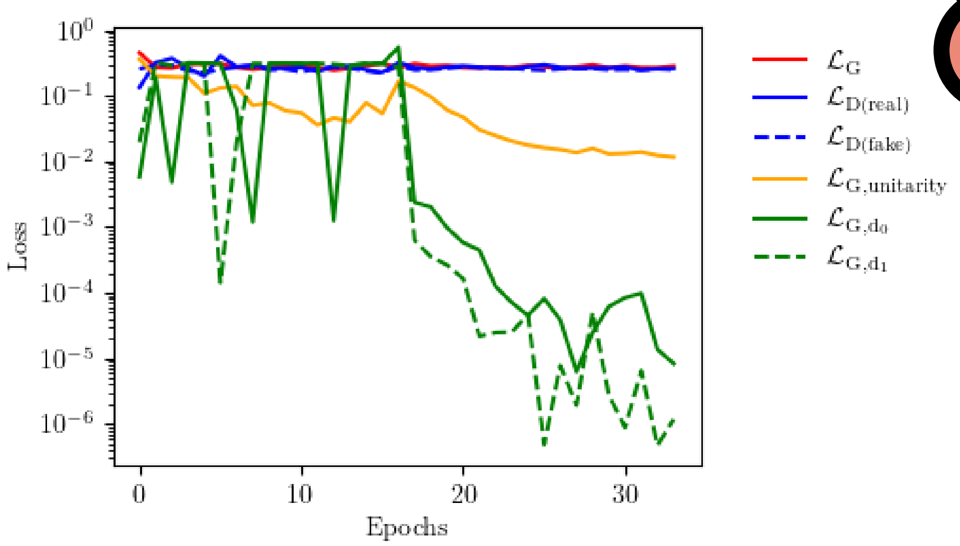




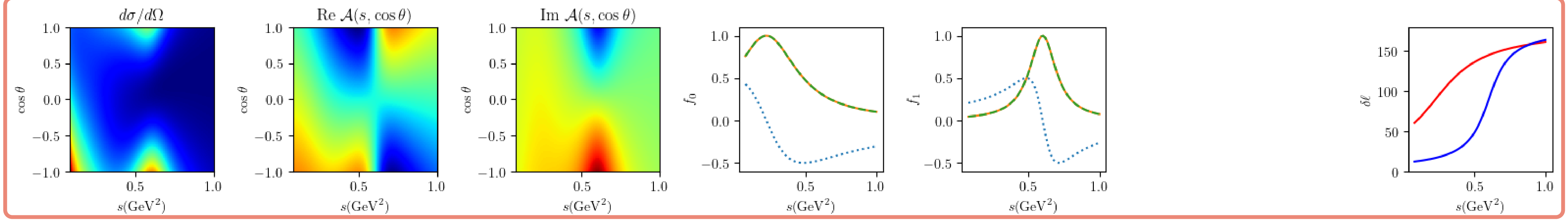
generated ("fake")

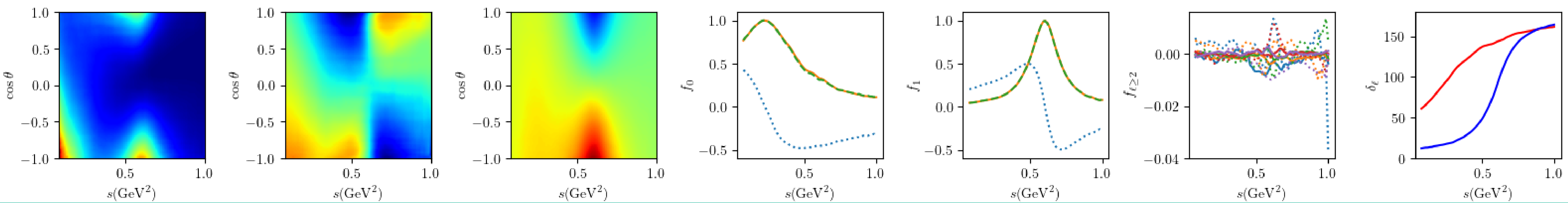
PRELIMINARY RESULTS

- Example of converged GAN with std=0.01:



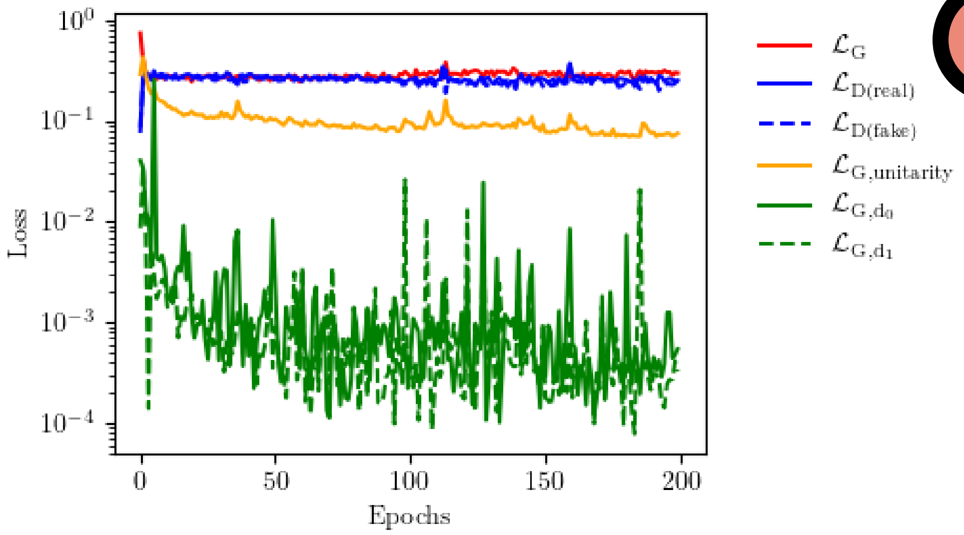
model ("true" without noise)





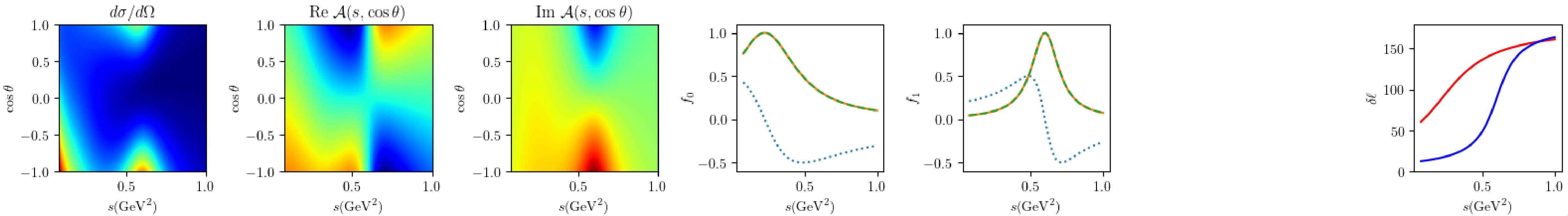
generated ("fake")

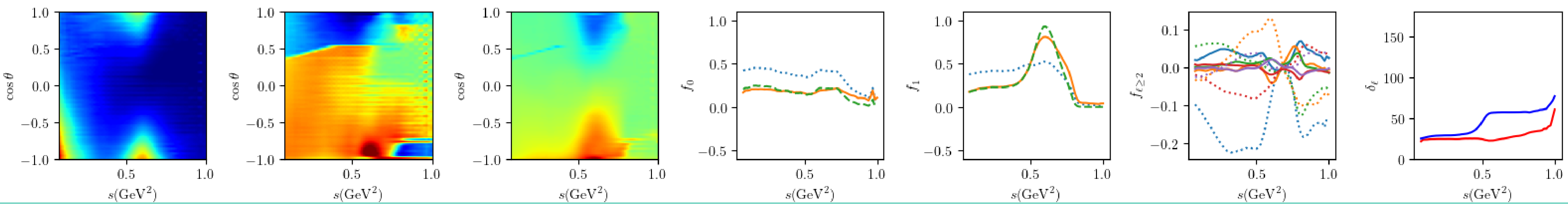
PRELIMINARY RESULTS



Example of non-converged GAN with std=0.01:

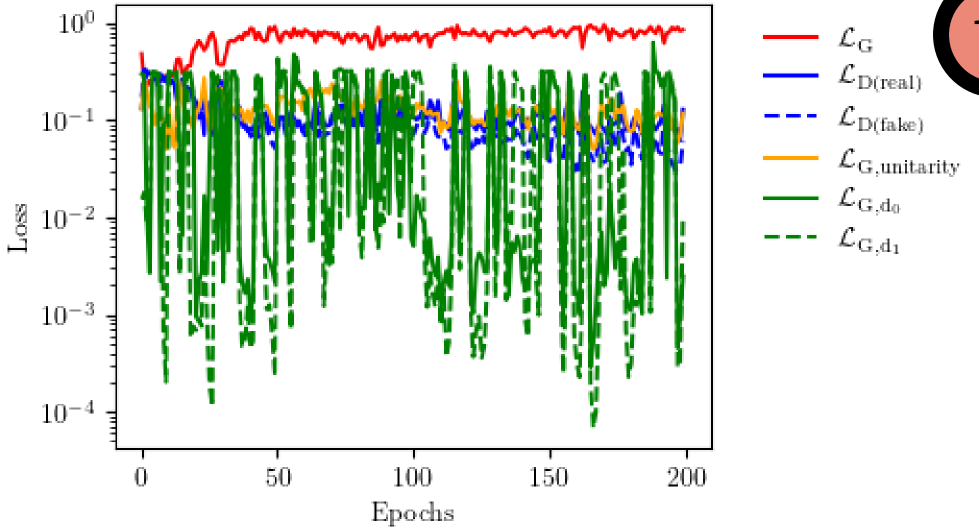
model ("true" without noise)





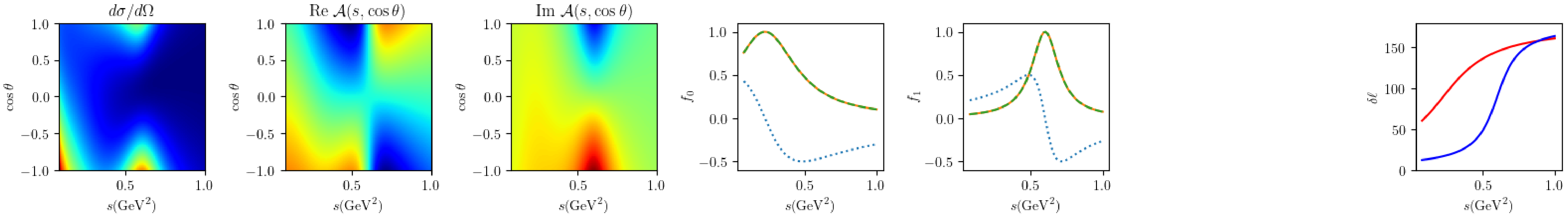
generated ("fake")

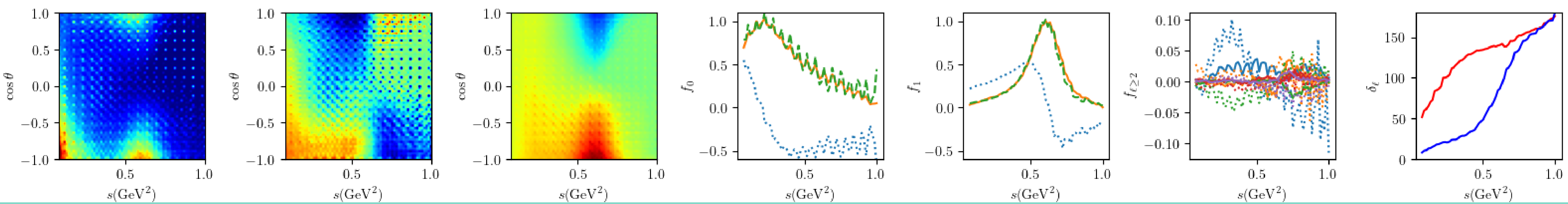
PRELIMINARY RESULTS



- Example of a “not too bad” non-converged GAN with std=0.05:

model (“true” without noise)





generated (“fake”)

CONCLUSIONS & OUTLOOK

Current achievements:

We developed a physics-constrained GAN to extract complex amplitudes from cross-section data.

The unitarity loss together with constraints on the phase allows us to recover the amplitude.

What's next?

Optimize the GAN architecture and the hyperparameters.

Explore additional/alternative physics-informed constraints to further stabilize the GAN training.

Perform a quantitative analysis and error estimation.

Future directions:

Extension to the event level using, e.g. normalizing flows.

Extension to more complicated processes and generalization of the physics constraints.

Preliminary status, but the results of using physics-constrained GANs to extract amplitudes from cross sections employing physics constraints are promising.