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Field Matching: an Electrostatic Paradigm to Generate and Transfer Data

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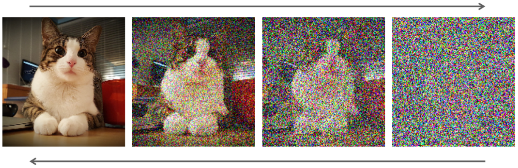
Physics-inspired generative models

Diffusion Models(DM) are based on thermodynamics and described by the forward and backward dynamics as:

$$dx_t = f(x_t, t)dt + g(t)dw_t \tag{1}$$

$$dx_t = (f(x_t, t) - g^2(t)s_\theta(x_t, t))dt + g(t)d\bar{w}_t \tag{2}$$

where $s_\theta(x_t, t))$ is an approximation of $\nabla_x \log p_t(x_t)$.



The **forward** process (1) describes diffusion stochastic process that corrupts data, injecting Gaussian pure noise.

The **backward** process (2) describes diffusion stochastic process that recovers data from Gaussian noise.

Are there other generative models based on principles of physics?

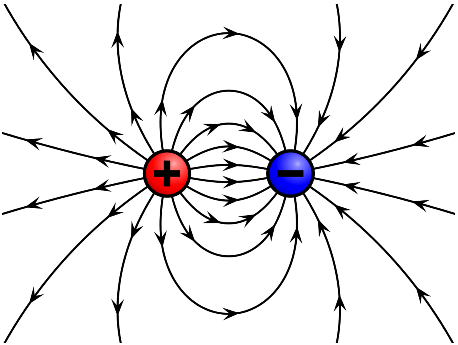
Maxwell's electrostatics

The point charge q at a point $\mathbf{x}'$ creates electric field:

$$\mathbf{E}(\mathbf{x}) = \frac{q}{4\pi} \frac{\mathbf{x} - \mathbf{x}'}{||\mathbf{x} - \mathbf{x}'||^3}. \tag{3}$$

The electric field from a charge distribution q(x) is found with the superposition principle as follows:

$$\mathbf{E}(\mathbf{x}) = \int \frac{1}{4\pi} \frac{(\mathbf{x} - \mathbf{x}')}{||\mathbf{x} - \mathbf{x}'||^3} q(\mathbf{x}') d\mathbf{x}'. \tag{4}$$



An **electric strength line** of the field $\mathbf{E}(\mathbf{x})$ is a curve $x(t)$ whose tangent to each point is parallel to the electric field. Thus, the motion along the field is represented as:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{E}(\mathbf{x}(t)), \tag{5}$$

The electric field flux

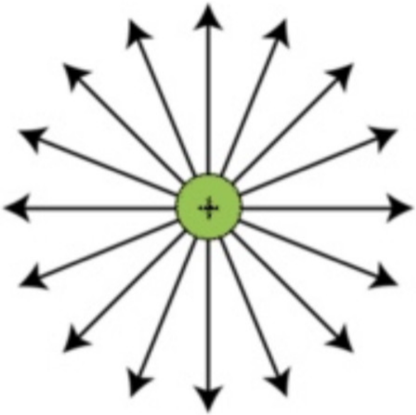
The **field flux** of $\mathbf{E}(\mathbf{x})$ through a surface Σ is defined as:

$$\Phi = \iint_{\Sigma} d\Phi = \iint_{\Sigma} \mathbf{E} \cdot \mathbf{dS}, \tag{6}$$

where $\mathbf{dS}$ is an area element of the finite surface Σ.

The **flux of electric field** Φ indicates the density of field lines passing through the finite surface Σ.

If we consider a point charge q, then the density of field lines is uniform through a spherical surface with q at its center as depicted in the figure



Poisson Flow Generative Model (PFGM)

We consider D-dimensional data distibution $\mathbb{P}_0(\cdot)$ whose samples $\widetilde{x} \sim \mathbb{P}_0(\cdot)$ located on a plane $z = 0$:

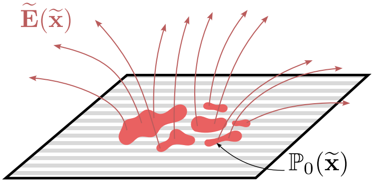
$$(x_1, x_2, \dots, x_D, z) = (\mathbf{x}, z) = \widetilde{\mathbf{x}} \in \mathbb{R}^{D+1}. \tag{7}$$

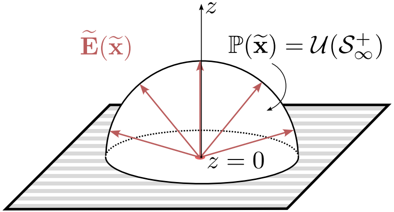
We interpret that $\widetilde{\mathbf{x}}$ are positive charges that create electric field $\widetilde{E}(\widetilde{\mathbf{x}})$ whose flux through plane $z = 0$ equals to $\mathbb{P}_0$.

If we move away from z $= 0$ to infinity, then the field of the charged plane is the field of a point charge.:

$$\mathbb{P}_\infty = \mathcal{U}(\mathcal{S}^+_\infty).$$

The electric field lines define the correspondence between easy-sampled distribution and untractable distribution.





The main goal is to approximate the field by a neural network and reverse dynamics.

$$d\widetilde{\mathbf{x}}(t) = -f_\theta(\widetilde{\mathbf{x}}(t))dt, \quad f_\theta(\cdot) \approx \widetilde{E}(\cdot) \tag{8}$$

Electrostatic Field Matching (EFM): Distributions

We develop **EFM** methodology suitable to **both** noise-to-data and data-to-data scenarios unlike PFGM.

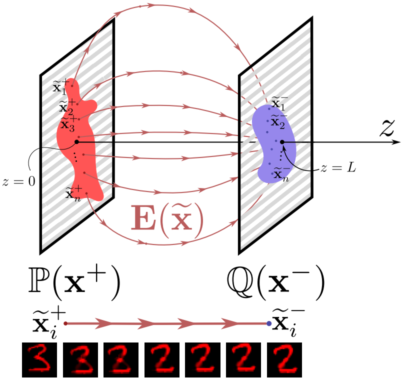
We consider distributions as charge densities and assign:

- $\mathbb{P}(\mathbf{x}^+)$ as a distribution of positive charges, $\mathbf{x}^+ \in \mathbb{R}^D$
- $\mathbb{Q}(\mathbf{x}^-)$ as a distribution of negative charges, $\mathbf{x}^- \in \mathbb{R}^D$

We augment $\mathbf{x}^+$ and $\mathbf{x}^-$ with $z=0$ and $z=L$:

$$q^+(\widetilde{\mathbf{x}}) = q^+(\mathbf{x}, z) = q^+(\mathbf{x})\delta(z), \quad q^+(\mathbf{x}) = \mathbb{P}(\mathbf{x}),$$

$$q^-(\widetilde{\mathbf{x}}) = q^-(\mathbf{x}, z) = q^-(\mathbf{x})\delta(z-L), \quad q^-(\mathbf{x}) = -\mathbb{P}(\mathbf{x}); (9)$$



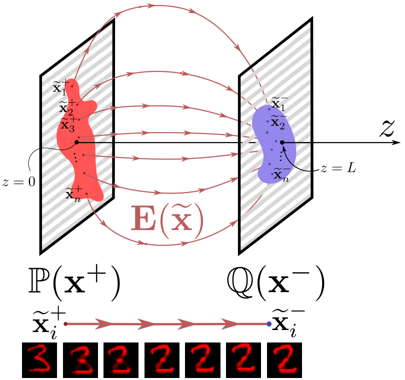
Electrostatic Field Matching (EFM): Field

Since each plate creates own field in a point $\widetilde{\mathbf{x}} \in \mathbb{R}^{D+1}$, then we use **Superpoisition principle** to define total field:

$$\mathbf{E}(\widetilde{\mathbf{x}}) = \mathbf{E}_{+}(\widetilde{\mathbf{x}}) + \mathbf{E}_{-}(\widetilde{\mathbf{x}}). \tag{10}$$

In accordance with Coulomb's law, the exact expression of each summand is defined as follows:

$$\mathbf{E}_{\pm}(\widetilde{\mathbf{x}}) = \int \frac{1}{S_D} \frac{\widetilde{\mathbf{x}} - \widetilde{\mathbf{x}}'}{||\widetilde{\mathbf{x}} - \widetilde{\mathbf{x}}'||^{D+1}} q^{\pm}(\widetilde{\mathbf{x}}') d\widetilde{\mathbf{x}}'. \tag{11}$$



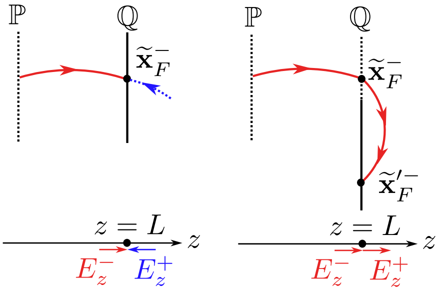
Again, the main goal is to approximate field by a neural network.

Electrostatic Field Matching (EFM): Field lines

From **Gauss's law** it follows that the lines originate from positive and terminate on negative charges

However, there are 2 scenarios with lines:
- a line terminates to the left of plate
- a line terminates to the right of plate

Moving along field lines from $\mathbb{P}$ to $\mathbb{Q}$:
- We stop on the second plate if $E_z^{\pm}(\widetilde{\mathbf{x}})$ have opposite sign
- We continue motion behind $\mathbb{Q}$ if $E_z^{\pm}(\widetilde{\mathbf{x}})$ have same sign



Having learned the electric field, we define map T that transform from $\mathbb{P}$ to $\mathbb{Q}$ and takes into account the aforementioned issues (see Th.3.1)

Electrostatic Field Matching (EFM): Training and Sampling

To define intermediate points $\widetilde{\mathbf{x}}$ between plates, we use uniform scheduler and add noise as follows:

$$\widetilde{\varepsilon} = ||\varepsilon|| \frac{m}{||m||}, \quad m \sim \mathcal{N}(0, I), \quad \varepsilon \sim \mathcal{N}(\frac{L}{2}, \sigma^2 I)$$

We learn a normalized field between the plates to provide stabil- ity of training procedure and fast convergence.

Having trained the normalized vector field $\frac{\mathbf{E}(\cdot)}{||\mathbf{E}(\cdot)||}$ in the extended space by $f_\theta(\cdot)$, we sample from $\mathbb{Q}(\mathbf{x}^-)$ as follows:

$$d\widetilde{\mathbf{x}} = d(\mathbf{x}, z) = \Big(\frac{d\mathbf{x}}{dt}\frac{dt}{dz}dz, dz\Big) = (\mathbf{E}_x(\widetilde{\mathbf{x}})\mathbf{E}_z^{-1}(\widetilde{\mathbf{x}}), 1)dz$$

$$= \Big(\frac{\mathbf{E}_x(\widetilde{\mathbf{x}})}{||\mathbf{E}(\widetilde{\mathbf{x}})||}\frac{||\mathbf{E}(\widetilde{\mathbf{x}})||}{\mathbf{E}_z(\widetilde{\mathbf{x}})}, 1\Big)dz \approx (f_\theta(\widetilde{\mathbf{x}})_x f_\theta^{-1}(\widetilde{\mathbf{x}})_z, 1)dz$$

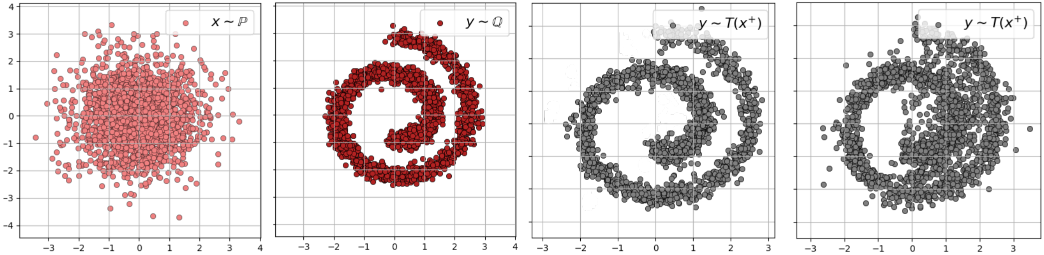
Algorithm 1 EFM Training

Input: Distributions accessible by samples:
$\mathbb{P}(\mathbf{x}^+)\delta(z)$ and $\mathbb{Q}(\mathbf{x}^-)\delta(z-L)$;
NN approximator $f_\theta(\cdot) : \mathbb{R}^{D+1} \to \mathbb{R}^{D+1}$;
Output: The learned electrostatic field $f_\theta(\cdot)$
Repeat until converged :
Sample a batch of points $\widetilde{\mathbf{x}}^+ \sim \mathbb{P}(\mathbf{x}^+)\delta(z)$;
Sample a batch of points $\widetilde{\mathbf{x}}^- \sim \mathbb{Q}(\mathbf{x}^-)\delta(z-L)$;
Sample a batch of times $t \sim \mathcal{U}(0, L)$;
Sample a batch of noise $\widetilde{\varepsilon}$ with (21);
Calculate $\widetilde{\mathbf{x}} = t\widetilde{\mathbf{x}}^+ + (1-t)\widetilde{\mathbf{x}}^- + \widetilde{\varepsilon}$;
Estimate $\mathbf{E}_+(\widetilde{\mathbf{x}})$ and $\mathbf{E}_-(\widetilde{\mathbf{x}})$ through (9);
Calculate $\mathbf{E}(\widetilde{\mathbf{x}})$ with (13);
Compute $\mathcal{L} = \mathbb{E}_{\widetilde{\mathbf{x}}}||f_\theta(\widetilde{\mathbf{x}}) - \frac{\mathbf{E}(\widetilde{\mathbf{x}})}{||\mathbf{E}(\widetilde{\mathbf{x}})||}||_2^2 \to \min_\theta$;
Update θ by using $\frac{\partial \mathcal{L}}{\partial \theta}$;

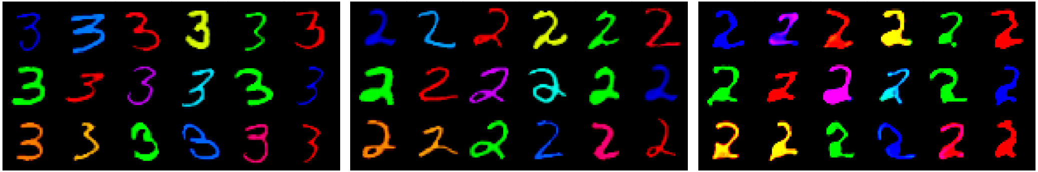
Algorithm 2 EFM Sampling

Input: sample $\tilde{\mathbf{x}}^+$ from $\mathbb{P}(\mathbf{x}^+)\delta(z)$; step size $\Delta\tau > 0$;
the learned field $f_\theta^*(\cdot) : \mathbb{R}^{D+1} \to \mathbb{R}^{D+1}$;
Output: mapped sample $\tilde{\mathbf{x}}^-$ approximating $\mathbb{Q}(\mathbf{x}^-)\delta(z-L)$
Set $\tilde{\mathbf{x}}_0 = \tilde{\mathbf{x}}^+$
for $\tau \in \{0, \Delta\tau, 2\Delta\tau, \dots, L-\Delta\tau\}$ **do**
Calculate $f_\theta^*(\tilde{\mathbf{x}}_\tau) = (f_\theta^*(\tilde{\mathbf{x}}_\tau)_x, f_\theta^*(\tilde{\mathbf{x}}_\tau)_z)$
$\tilde{\mathbf{x}}_{\tau+\Delta\tau} = \big[(\tilde{\mathbf{x}}_\tau)_x + f_\theta^*(\tilde{\mathbf{x}}_\tau)_z^{-1} f_\theta^*(\tilde{\mathbf{x}}_\tau)_x \Delta\tau; \tau + \Delta\tau\big]$

Electrostatic Field Matching (EFM): Translating Experiments



(a) $\mathbb{P}(\mathbf{x}^+)$ samples. **(b)** $\mathbb{Q}(\mathbf{x}^-)$ samples. **(c)** Map $T(\mathbf{x}^+)$ with $L = 6$. **(d)** Map $T(\mathbf{x}^+)$ with $L = 30$.

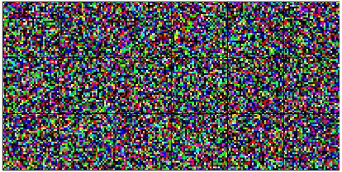


(a) Samples from $\mathbb{P}(\mathbf{x}^+)$, which are placed on the left plate $z = 0$.

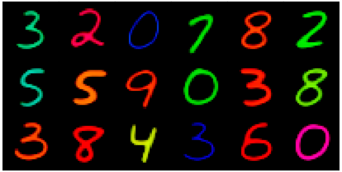
(b) Samples from **our** approximation of $\mathbb{Q}(\mathbf{x}^-)$, located on the right plate $z = 10$.

(c) Samples from **FM**'s approximation of $\mathbb{Q}(\mathbf{x}^-)$, located on the right plate $z = 10$.

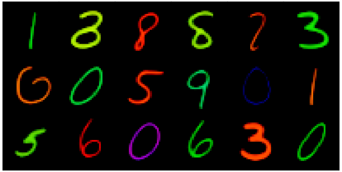
Electrostatic Field Matching (EFM): Image Generation



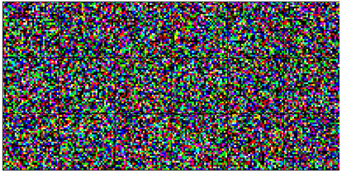
(a) White noise samples from $\mathbb{P}(\mathbf{x}^+)$, which are placed on the left plate $z = 0$.



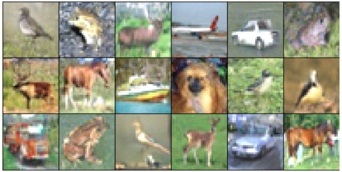
(b) Samples from **our** approximation of $\mathbb{Q}(\mathbf{x}^-)$, located on the right plate $z = 30$.



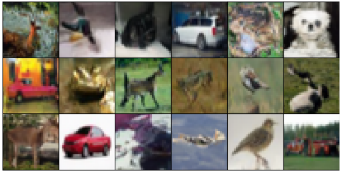
(c) **PFGM**'s approximation of $\mathbb{Q}(\mathbf{x}^-)$, simulated from hemisphere.



(a) White noise samples from $\mathbb{P}(\mathbf{x}^+)$ which are placed on the left plate $z = 0$.



(b) **Our** approximation of $\mathbb{Q}(\mathbf{x}^-)$ located on the right plate $z = 500$.

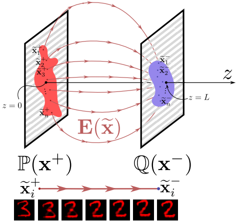


(c) **PFGM**'s approximation of $\mathbb{Q}(\mathbf{x}^-)$ simulated from hemisphere.

Thank you

Field Matching: an Electrostatic Paradigm to Generate and Transfer Data

The novel electrostatic based methodology for noise-to-data and data-to-data scenarios.



GitHub

https://github.com/justkolesov/FieldMatching