Field Matching: an Electrostatic Paradigm to Generate and Transfer Data

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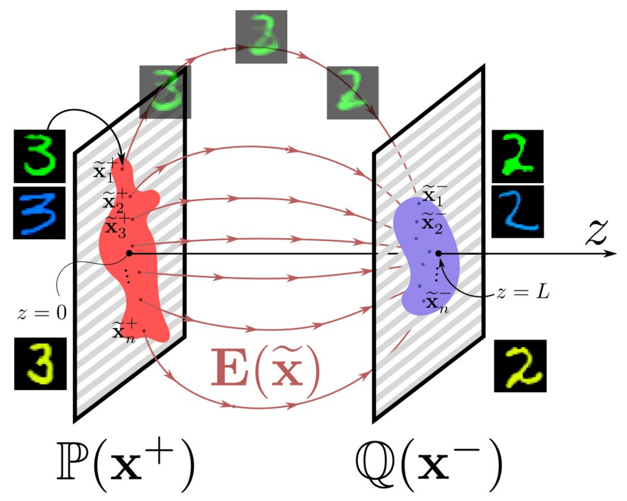
Overview

Our **idea** is to consider distributions as electric charge densities, placed on plates of capacitor.

- Take 2 any data distributions $\mathbb{P}(\mathbf{x})$ and $\mathbb{Q}(\mathbf{x})$
- Assign samples from $\mathbb{P}(\mathbf{x})$ as positive charges
- Assign samples from $\mathbb{Q}(\mathbf{x})$ as negative charges
- Choose the distance L between plates
- Place $\mathbb{P}(\mathbf{x}^+)$ and $\mathbb{Q}(\mathbf{x}^-)$ on these plates
- Define **Ground-truth** field via Coulomb's law
- Approximate the field by Neural net
- Simulate sampling from one plate to another



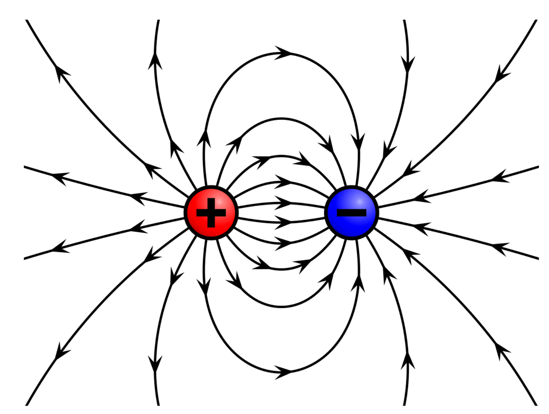
Maxwell's electrostatics

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

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

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

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



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:

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

The electric field flux

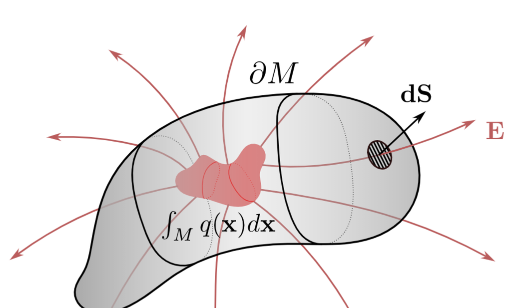
The **field flux** of E(x) through a surface Σ is defined as:

$$\Phi = \iint_{\Sigma} d\Phi = \iint_{\Sigma} \mathbf{E}\cdot d\mathbf{S}, \qquad (1)$$

where **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 Models[1]

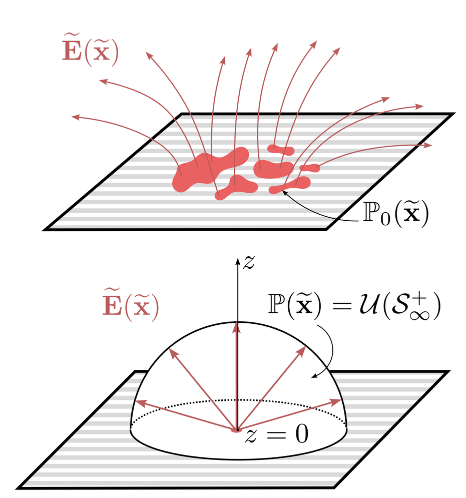
D-dimensional distibution $\mathbb{P}_0(\cdot)$ is considered whose samples $\widetilde{x}$ located on plane $z=0$:

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

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

If we move away from z = 0 to infinity, then the field of plane is 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.

[1] - Xu, Y., Liu, Z., Tegmark, M., Jaakkola, T. (2022). Poisson flow generative models. Advances in Neural Information Processing Systems, 35, 16782-16795.

Our methodology

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

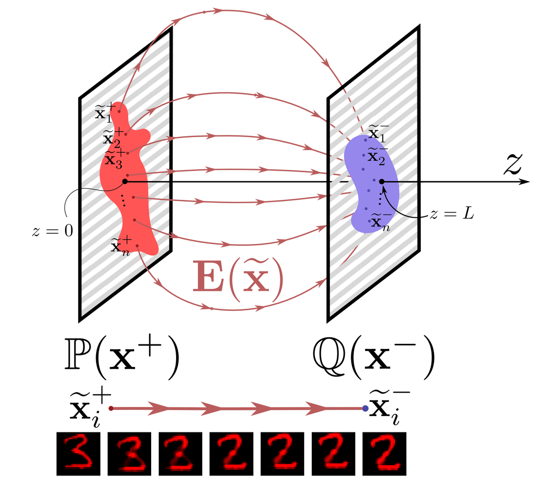
We consider distributions as charge densities:

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

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

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

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



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 in this interplate point:

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

In accordance with Coulomb's law, the exact expression of each summand is defined via the follwoing formulation, where S_D is D-dimensional unit sphere:

$$\mathbf{E}_\pm(\widetilde{\mathbf{x}}) = \int \frac{1}{S_D}\frac{\widetilde{\mathbf{x}}-\widetilde{\mathbf{x}}'}{||\widetilde{\mathbf{x}}-\widetilde{\mathbf{x}}'||^{D+1}} q^\pm(\widetilde{\mathbf{x}}')d\widetilde{\mathbf{x}}'. \qquad (2)$$

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

Algorithm

To better approximate the **Ground-truth** field between plates by neural-network, it is necessary to choose appropriate inter-plate points. In our paper, we use linear interpolation as $\widetilde{\mathbf{x}} = t\widetilde{\mathbf{x}}^+ + (1-t)\widetilde{\mathbf{x}}^- + \widetilde{\varepsilon}$, where $\widetilde{\varepsilon}$ is a noise. This approach is one of possible ways to determine intermediate points and is not connected to **Flow Matching**.

Algorithm 1 EFM Training

```
1: procedure Training stage
   Input: Distributions accessible by samples:  P(x+)δ(z) and Q(x−)δ(z − L);
     NN approximator f_θ(·) : R^{D+1} → R^{D+1};
2: Output: The learned electrostatic field f_θ(·).
3: Repeat until converged :
4:     Sample a batch of points x̃+ ∼ P(x+)δ(z)
5:     Sample a batch of points x̃− ∼ Q(x−)δ(z − L)
6:     Sample a batch of times t ∼ U(0, L)
7:     Sample a batch of noise ε̃
8:     Calculate x̃ = t x̃+ + (1 − t) x̃− + ε̃
9:     Estimate E+(x̃) and E−(x̃) by (2)
10:    Calculate E(x̃) by Superposition principle.
11:    Compute L = E_x̃ ||f_θ(x̃) − E(x̃)/||E(x̃)|| ||²_2 → min_θ
12:    Update θ by using ∂L/∂θ
13: end procedure
```

Algorithm 2 EFM Sampling

```
1: procedure Inference
2: Input: Sample x̃+ from P(x+)δ(z); step size Δτ > 0;
     the learned field f*_θ(·) : R^{D+1} → R^{D+1}; .
3: Output: mapped sample x̃− approximating Q(x−)δ(z − L).
4: Set: x̃_0 = x̃+ .
5: for τ ∈ {0, Δτ, 2Δτ, ..., L − Δτ} do
6:     Calculate f*_θ(x̃_τ) = (f*_θ(x̃_τ)_x, f*_θ(x̃_τ)_z)
7:     x̃_{τ+Δτ} = [(x̃_τ)_x + f*_θ(x̃_τ)_z^{-1} f*_θ(x̃_τ)_x Δτ; τ + Δτ]
8: x̃− ← x̃_L
9: end procedure
```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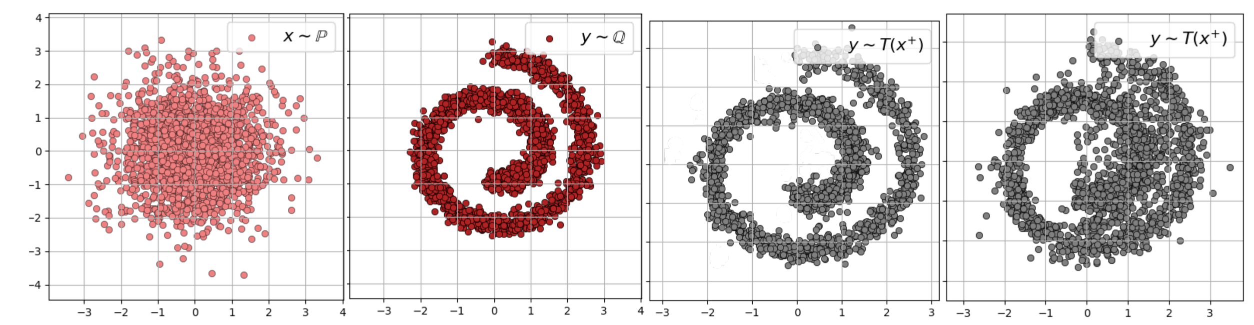
Toy experiments

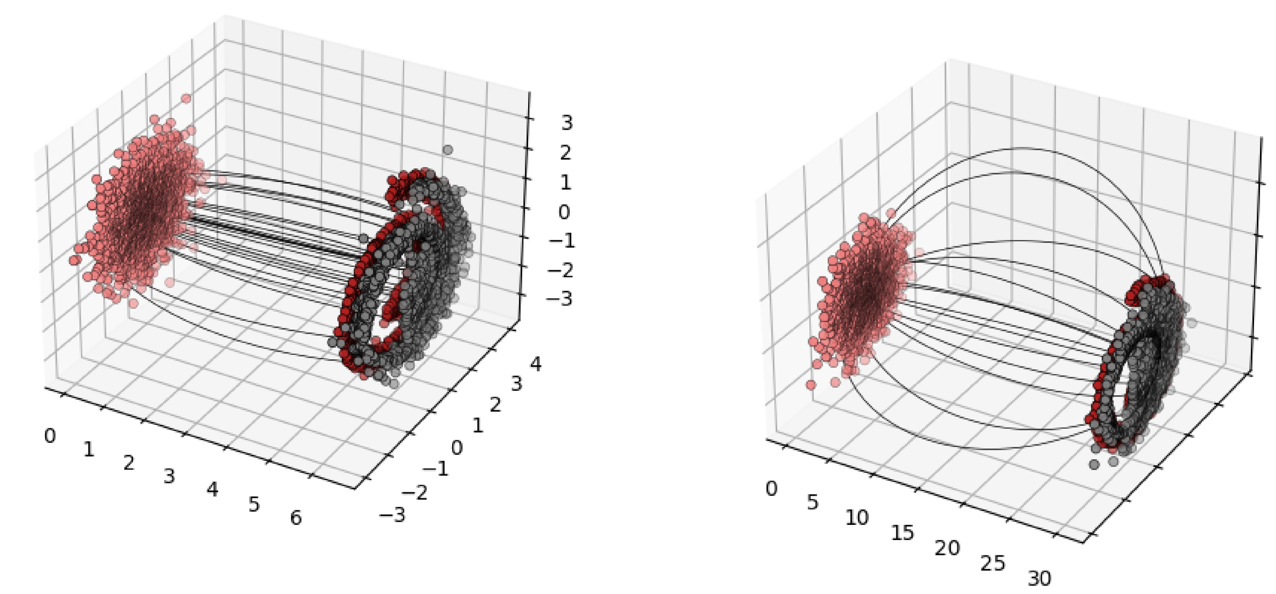


(a) $\mathbb{P}(\mathbf{x}^+)$ samples. (b) $\mathbb{Q}(\mathbf{x}^-)$ samples. (c) Map $T(\mathbf{x}^+)$, $L=6$. (d) Map $T(\mathbf{x}^+)$, $L=30$.

We consider $\mathbb{P}(\mathbf{x})$ as a zero-mean Gaussian distribution and $\mathbb{Q}(\mathbf{x})$ as Swiss-roll.

The distance L between plates of D-dimensional capacitor is the **crucial** hyper-parameter that has signifact influence to our's method performance.

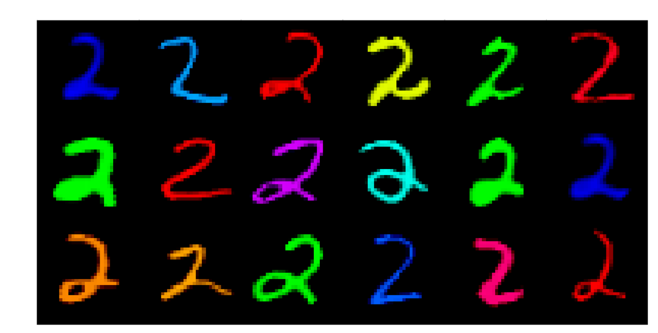
- When L is small, mapping recovers accurately (Fig. c)
- When L is large, mapping recovers poorly (Fig. d)



Data-to-Data scenario

We consider unpaired translation task between colored digits. We assign colored digits 3 as positive charges and digits 2 as negative. We demonstrate that **our** method accurately recovers the target distribution, preserving perfectly colors of initial digits.

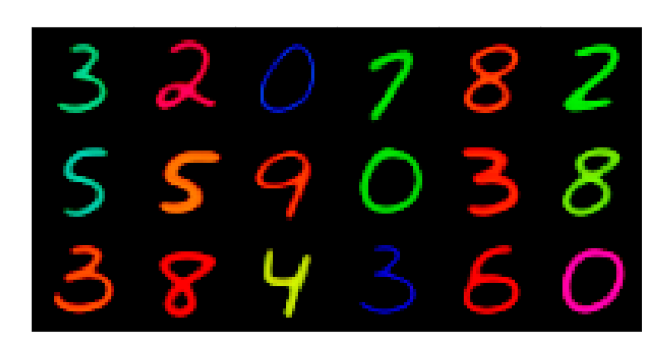
(g) Samples from $\mathbb{P}(\mathbf{x}^+)$ from $z=0$



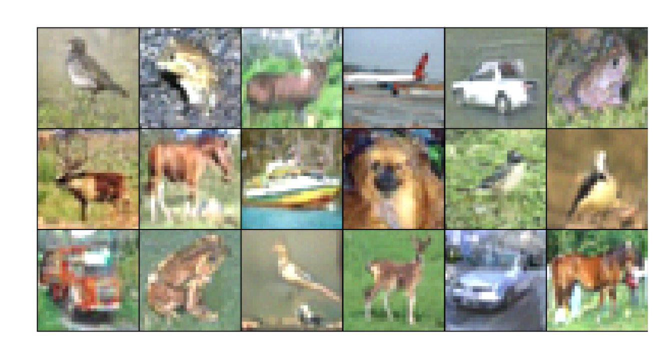
(h) Samples of **our** approx. of $\mathbb{Q}(\mathbf{x}^-)$ from $z=10$.

Noise-to-Data scenario

We also consider unconditional generation task with CIFAR-10 dataset and colored digits. We place white noise on the left plate and samples from datasets to the right. We see that our method acccurately recovers the initial distribution.



(i) Samples of **our** approx. of colored digits.



(j) Samples from **our** approx. of CIFAR-10.

Conclusion

We developed the novel physics-inpired generative model that is adopted for **both** scenarios: noise-to-data and data-to-data.

GitHub

https://github.com/justkolesov/FieldMatching