Discretize mean-field limit using JKO, see if it is similar to GD.

Mean-field limit(Chizat & Bach): For a sufficiently large width, the training dynamics of a NN can be coupled with the evolution of a probability distribution described by a PDE. **Pros:** Using a smaller initialization scale than in the NTK regime, feature learning is allowed to happen. **Cons:** Discretization is not trivial, and PDE are a bit harder than linear models. The theory is lacking a lot of useful results.

- Block: obligé de modifier l'algo du papier pour que ça converge, on sait plus trop se qu'il se passe (potentiellement on fait une GD..)
- Next step: donner une initialisation spécifique (uniquement une activation) et voir si ça se diffuse en suivant les coûts. Utiliser JKOnet pour tester aussi.

1 Classic setup

Data $x_i \in \mathbb{R}^d$ and labels $y_i \in \mathbb{R}$, j = 1,...,n

First layer $w_i \in \mathbb{R}^d$, second layer $\alpha_i \in \mathbb{R}$, i = 1,...,m

 $\gamma > 0$ step-size, β regularization

$$\mathcal{L}(W,\alpha) = \sum_{j=1}^{n} \left(\underbrace{\sum_{i=1}^{m} \max(0, w_i^{\top} x_j) \alpha_i - y_j}^2 + \lambda \underbrace{\sum_{i=1}^{m} \|w_i\|_2^2 + \alpha_i^2}_{\text{Weight Decay}} \right)$$

Discret time.

Full-batch gradient descent

$$(W, \alpha)_{t+1} = (W, \alpha)_t - \gamma \nabla \mathcal{L}((W, \alpha)_t)$$

Implicit

$$\theta_{t+1} = \underset{\theta}{\operatorname{arg\,min}} \mathcal{L}(\theta) + \frac{1}{2\gamma} \|\theta - \theta_t\|$$

Continuous time.

Taking $\gamma \to 0$, we get the gradient flow: $\frac{d\theta_t}{dt} = -\nabla \mathcal{L}(\theta_t)$. We make ReLU differentiable with $\sigma'(0) = 0$ as justified in (Boursier et al.).

2 Using a measure

$$\int_{\Theta} m(\theta; x) d\mu(\theta) = \frac{1}{m} \sum_{i=1}^{m} \langle w_i, x_j \rangle_{+} \alpha_i$$

Different ways to use a measure:

- $\Theta = \mathbb{R}^d \times \mathbb{R}$, measure $\mu = \frac{1}{m} \sum_{i=1}^m \delta_{\theta_i = (w_i, \alpha_i)}$, output of one neuron $m(\theta = (w, \alpha); x) = \langle x, w \rangle_+ \alpha$: (works, output matches discrete)
- $\Theta = \mathbb{R}^d$, measure $\mu = \frac{1}{m} \sum_{i=1}^m \alpha_i \delta_{\theta_i = w_i}$ output of one neuron $m(\theta = w; x) = \langle x, w \rangle_+$ (works)
- $\Theta = \mathbb{R}^d \times \mathbb{R}^d$, output of one neuron $m(\tilde{w}_+, \tilde{w}_-, x) = \langle \tilde{w}_+, x \rangle \langle \tilde{w}_-, x \rangle$ (works, separate neg and positive)
- $\Theta = (S^{d-1} \times \mathbb{R})$, output of one neuron $m((d, \tilde{\alpha}); x) = \tilde{\alpha} \langle d, x \rangle = \tilde{\alpha} \mathbb{1}_{\langle d, x \rangle > 0}$ (works), mapping: $d = \frac{w}{\|w\|}$ and $\tilde{\alpha} = \|w\|\alpha$. Gradient are not equal to discrete.

2.1 Algorithm, discretize the measure's space

Take a grid of N points in Θ , we can match the notation above by taking a neuron for each point of the grid m = N.

$$\mu(t+1) = \underset{\mu \in \mathcal{M}(\Theta)}{\arg\min} F(\mu) + \frac{1}{2\gamma} W_2(\mu; \mu(t))$$

A essayer: KL à la place de distance wasserstein.

Remark: le 1/m c'est principalement pour être ok à l'infini. Dans le papier JKO (Carlier et al.) ils utilisent un vecteur de proba

2.2 Infinity and beyond

Take $\gamma \to 0$, get gradient flow. Take $m \to \infty$, get wasserstein gradient flow (Bach & Chizat), and if it converges, it goes to the global optimal.

2.3 JKO

Use something out of the box to compute JKO flow

- Meta Optimal Transport (paper) and (code git): InputConvexNN to predict solution of OT problem
- JKOnet (paper) and (code git):
 - /models -> sinkhorn loss defined in loss.py, differentiable loop in fixed point.py
 - next step: trying to create the right Geometry object from OTT library, which is what's used for sinkhorn
 - Or try to use the whole thing?

2.3.1 Grid Problems

The grid currently dictate the neuron's scale, giving multiple choices. One solution: duplicate each neuron, make one with a small scale and one with a very big scale.

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