Lecture 22, Monday, 5/16/2022

Today: Convergence of the JKO scheme.

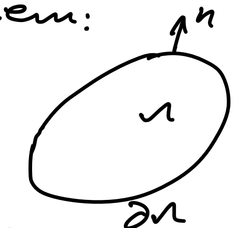
<u>The heat equation</u> $\partial_t u = \Delta u \qquad u = u(x,t)$

Given: $\Omega \subseteq \mathbb{R}^d$, bounded and smooth domain

$u_0 = u_0(x)$, bounded and smooth function.

The initial-boundary-value problem:

$$\begin{cases} \partial_t u = \Delta u & \Omega \times (0,\infty) \\ \partial_n u = 0 & \partial\Omega \times (0,\infty) \\ u(\cdot, 0) = u_0 & \end{cases}$$




$\partial_n u = (\nabla \cdot n) u$

The gradient flow: $\partial_t u = -\delta I[u]$.

$$I[v] := \int_\Omega \frac{1}{2} |\nabla v|^2 dx, \quad \delta I[v] = -\Delta v.$$

<u>The implicit Euler scheme</u> Let $\tau > 0$, $t_k = k\tau$.

$$u_k = u_k^\tau \approx u(\cdot, t_k): \begin{cases} u_0 : \text{given} \\ \dfrac{u_{k+1} - u_k}{\tau} = \Delta u_{k+1} \quad (k = 0, 1, \cdots) \end{cases}$$

$$u_{k+1} = \operatorname*{argmin}_u \left( \frac{1}{2\tau} \|u - u_k\|^2_{L^2(\Omega)} + I[u] \right), \text{ unique}$$

<u>The JKO scheme</u> Define

$$F(\rho) = \int_\Omega \rho \log \rho \, dx, \qquad \rho = \rho(x) \geq 0, \ x \in \Omega.$$

$$\mathcal{P}(\Omega) = \{ \rho \in L^1(\Omega) : \rho \geq 0, \int_\Omega \rho dx = 1 \}. \qquad \rho \in \mathcal{P}(\Omega) \Rightarrow \int_\Omega |x|^2 \rho(x) dx < \infty$$

Given: $\rho_0 \in \mathcal{P}(\Omega)$, $\tau > 0$, $t_k = k\tau$, $k = 0, 1, 2, \cdots$

$$\rho_{k+1} = \operatorname*{argmin}_\rho \left( \frac{1}{2\tau} W_2^2(\rho, \rho_k) + F[\rho] \right)$$

Note: for $\xi, \eta \in \mathcal{P}(\Omega)$, $W_2(\xi, \eta) = W_2(\xi dx, \eta dx)$.

$X = \Omega$; compact, Euclidean distance.

Convergence: up to a subseq. $\rho^\tau \to \rho$ in $W_2$ and $\partial_t \rho = \Delta \rho$.

<u>The Fokker-Planck eq. (FPE):</u>

$$\partial_t \rho = \beta^{-1} \Delta \rho + \nabla \cdot (\rho \nabla V)$$

$V : \mathbb{R}^d \to \mathbb{R}$ given, bounded below.

Known: $\rho dx$ is the probability distribution for the stochastic process $X_t \in \mathbb{R}^d$:

$$dX_t = -\nabla V(X_t) dt + \sqrt{2\beta^{-1}}\, dW_t$$

Here: $W_t$ is the standard $d$-dimensional Brownian motion.

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Today: Proof of convergence $\rho^\tau \xrightarrow{W_2} \rho$.

We have proved (cf. last lecture): Given $\rho_k$

$$\exists ! \; \rho_{k+1} = \underset{\rho \in \mathcal{P}(\Omega)}{\operatorname{argmin}} \left( \frac{1}{2\tau} W_2^2(\rho, \rho_k) + F[\rho] \right),$$

where $F[\rho] = \int_\Omega \rho \log \rho \, dx$.

<u>Brenier's Theorem</u> Let $X = \mathbb{R}^d$ and $\mu, \nu \in \mathcal{P}_2(X)$ with $d\mu = g\, dx$ for some $g \in L^1(\mathbb{R}^d)$. Then, $\exists ! \; \bar{\gamma} \in \mathcal{A}(\mu, \nu)$ s.t. $W_2^2(\mu, \nu) = \int_{X \times X} \frac{1}{2} |x - y|^2 d\bar{\gamma}(x, y)$. Moreover, $\bar{\gamma} = (Id \times T)_\# \mu$ and $T = \nabla \varphi$ for some convex $\varphi$.

We will prove this theorem when we study the duality.

The minimizer $\hat{\rho}$ satisfies some minimality condition.

<u>Lemma</u> Let $\rho_0, \hat{\rho}$ be the same as above. Assume:

(1) $\xi \in C^\infty(\Omega, \mathbb{R}^d)$ is tangent to $\partial\Omega$;

(2) $T: \Omega \to \Omega$ is the optimal map from $\rho_0$ to $\hat{\rho}$.

Then $\displaystyle\int_\Omega \hat{\rho}\, \nabla\cdot\xi \, dx = \frac{1}{2\tau}\int_\Omega \langle \xi\circ T, T - Id\rangle \rho_0 \, dx.$

The idea is to perturb $\hat{\rho}$ and use the minimizer property of $\hat{\rho}$. This is similar to deriving the Euler-Lagrange eq. But the perturbation is done quitely differently. Sometimes, the method is called the method of <u>domain variations</u>.

<u>Proof of Lemma</u> Consider $\begin{cases} \dot{\Phi}(t,x) = \xi(\Phi(t,x)), \\ \Phi(0,x) = x. \end{cases}$

Since $\xi$ is tangential to $\partial\Omega$, $\Phi(t): \Omega \to \Omega$ is a diffeomorphism. Define $\rho_\varepsilon = \Phi(\varepsilon)_\# \hat{\rho} \in \mathcal{P}(\Omega)$.

[Note that $\varepsilon \in \mathbb{R}$ can be positive, negative, or 0. Note also that $\Phi(\varepsilon, x) = x + \varepsilon\,\xi(x) + O(\varepsilon^2)$ if $|\varepsilon| << 1$.] We have

$$\hat{\rho}(x) = \rho_\varepsilon(\Phi(\varepsilon,x))\det\nabla\Phi(\varepsilon,x). \qquad (*)$$

So, $\int_\Omega \rho_\varepsilon(y) \log \rho_\varepsilon(y)\,dy = \int_\Omega \log \rho_\varepsilon(y)\ \rho_\varepsilon(y)\,dy$

$$\overset{\rho_\varepsilon = \Phi(\varepsilon)\#\hat{\rho}}{=\!=\!=} \int_\Omega \log \rho_\varepsilon(\Phi(\varepsilon, x))\, \hat{\rho}(x)\,dx$$

$$\overset{(*)}{=\!=} \int_\Omega \hat{\rho}(x) \log \frac{\hat{\rho}(x)}{\det \nabla \Phi(\varepsilon, x)}$$

$$= \int_\Omega \hat{\rho}(x) \log \hat{\rho}(x)\,dx - \int_\Omega \hat{\rho}(x) \log \det \nabla\Phi(\varepsilon, x)\,dx$$

$$= \int_\Omega \hat{\rho}(x) \log \hat{\rho}(x)\,dx - \int_\Omega \hat{\rho}(x) \log(1 + \varepsilon \nabla\cdot\xi + o(\varepsilon))\,dx$$

$$= \int_\Omega \hat{\rho}(x) \log \hat{\rho}(x)\,dx - \varepsilon \int_\Omega \hat{\rho}(x)\ \nabla\cdot\xi\,dx + o(\varepsilon).$$

Now, let $\gamma \in \mathcal{A}(\hat{\rho}, \rho_0)$ s.t. $W_2^2(\hat{\rho}, \rho_0) = \int_{\Omega\times\Omega} |x-y|^2\,d\gamma(x,y)$.
Set $\gamma_\varepsilon = (\Phi(\varepsilon, \cdot) \times Id)\# \gamma \in \mathcal{A}(\rho_\varepsilon, \rho_0)$. Since $\Phi(\varepsilon, x) = x + \varepsilon\xi(x) + o(\varepsilon)$, we get

$$W_2^2(\rho_\varepsilon, \rho_0) \le \int_{\Omega\times\Omega} |x-y|^2\,d\gamma_\varepsilon(x,y) = \int_{\Omega\times\Omega} |\Phi(\varepsilon,x) - y|^2\,d\gamma(x,y)$$

$$= \int_{\Omega\times\Omega} \left[|x-y|^2 + 2\varepsilon \langle \xi(x), x-y\rangle + o(\varepsilon)\right] d\gamma(x,y)$$

$$= W_2^2(\hat{\rho}, \rho_0) + 2\varepsilon \int_{\Omega\times\Omega} \langle \xi(x), x-y\rangle\,d\gamma(x,y) + o(\varepsilon).$$

Therefore, since $\hat{\rho}$ is a minimizer,

$$\frac{W_2^2(\hat{\rho}, \rho_0)}{2\tau} + \int_\Omega \hat{\rho} \log \hat{\rho}\,dx \le \frac{W_2^2(\rho_\varepsilon, \rho_0)}{2\tau} + \int_\Omega \rho_\varepsilon \log \rho_\varepsilon\,dx$$

$$\le \frac{W_2^2(\hat{\rho}, \rho_0)}{2\tau} + \frac{\varepsilon}{\tau} \int_{\Omega\times\Omega} \langle \xi(x), x-y\rangle\,d\gamma(x,y)$$

$$+ \int_\Omega \hat{\rho} \log \hat{\rho}\,dx - \varepsilon \int_\Omega \hat{\rho}\ \nabla\cdot\xi\,dx + o(\varepsilon),$$

leading to

$$\varepsilon\left[\frac{1}{\tau}\int_{\Omega\times\Omega}\langle\xi(x), x-y\rangle\, d\gamma(x,y) - \int_\Omega \hat{\rho}\,\nabla\cdot\xi\, dx\right] + o(\varepsilon) \geq 0.$$

But $\varepsilon>0$, $\varepsilon<0$ possible. So,

$$\int_\Omega \hat{\rho}\,\nabla\cdot\xi\, dx = \frac{1}{\tau}\int_{\Omega\times\Omega}\langle\xi(x), x-y\rangle\, d\gamma(x,y).$$

If $T$ is the optimal transport map from $\rho_0$ to $\hat{\rho}$, with $\gamma = (T\times Id)\#\rho_0$, then

$$\int_{\Omega\times\Omega}\langle\xi(x), x-y\rangle\, d\gamma(x,y) = \int_\Omega \langle(\xi\circ T)(x), T(x)-x\rangle \rho_0(x)\, dx.$$

Hence, $\int_\Omega \hat{\rho}\,\nabla\cdot\xi\, dx = \frac{1}{\tau}\int_\Omega \langle \xi\circ T, T-Id\rangle \rho_0\, dx.$ <u>QED</u>

<u>Theorem</u> Let $\Omega\subseteq\mathbb{R}^d$ be a bounded and smooth domain. Let $\tau>0$ and $t_k = k\tau$ $(k=0,1,\cdots)$. Assume $\rho_0\in\mathcal{P}(\Omega)$ and $F[\rho_0] = \int_\Omega \rho_0\log\rho_0\, dx < \infty$. Let $\rho_{k+1}^\tau \in \mathcal{P}(\Omega)$ be the unique minimizer of

$$J_k[\rho] = \frac{1}{2\tau} W_2^2(\rho,\rho_k) + F[\rho]$$

among all $\rho\in\mathcal{P}(\Omega)$, $k=0,1,\cdots$. Let $\rho^\tau(t) = \rho_k^\tau$ if $t_k\leq t< t$. Then there exist $\rho\in L^1_{loc}([0,\infty)\times\Omega)$ and a subsequence of $\{\rho^\tau\}_{\tau>0}$, not relabeled, such that $\rho^\tau\to\rho$ weakly in $L_{loc}([0,\infty)\times\Omega)$. Further, $\rho$ is the distributional solution to the initial-boundary-value problem of the heat equation.

<u>Sketch of Proof</u> Need to show that

$$\int_\Omega \varphi \frac{\rho^\tau - \rho_0}{\tau} dx = \int_\Omega \Delta\varphi \rho^\tau + o(\tau) \quad \forall \varphi \in C_c^\infty(\Omega).$$

By the above lemma, with $\xi = \nabla\varphi$,

$$\int_\Omega \rho^\tau \Delta\varphi \, dx = \frac{1}{\tau}\int_\Omega \langle T - Id, \nabla\varphi \rangle \rho^\tau dx. \qquad (**)$$

Let $T_\# \rho^\tau = \rho_0$. Then

$$\int_\Omega \varphi \frac{\rho^\tau - \rho_0}{\tau} dx = \frac{1}{\tau}\int_\Omega \varphi \rho^\tau dx - \frac{1}{\tau}\int_\Omega \varphi \rho_0 \, dx$$

$$= \frac{1}{\tau}\int_\Omega \varphi \rho^\tau dx - \frac{1}{\tau}\int_\Omega (\varphi \circ T) \rho^\tau dx$$

$$= -\frac{1}{\tau}\int_\Omega (\varphi\circ T - \varphi)\rho^\tau dx$$

$$= -\frac{1}{\tau}\int_\Omega \int_0^1 \langle \nabla\varphi((1-t)x + t T(x)), T(x) - x \rangle dt \, \rho^\tau(x) dx$$

$$= -\frac{1}{\tau}\int_\Omega \int_0^1 \langle \nabla\varphi(x), T(x) - x\rangle \rho^\tau(x) dx + R(\tau)$$

$$\overset{(**)}{=} \int_\Omega \Delta\varphi \rho^\tau + R(\tau).$$

Moreover,

$$|R(\tau)| \le \frac{\mathrm{Lip}(\nabla\varphi)}{\tau}\int_\Omega \int_0^1 t |T(x) - x|^2 dt \, \rho^\tau(x) dx$$

$$= \frac{\mathrm{Lip}(\nabla\varphi)}{2\tau} W_2^2(\rho_0, \rho_\tau) = o(\tau). \quad \underline{\text{QED}}$$