DSC190: Machine Learning with Few Labels

A "standardized" view of ML

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Logistics

- HW1 due extended to Sunday (10/24)
- HW2 out: (much) easier than HW1 !
- Mid-term survey

Outline

- Functional derivative
- A "standardized" view of ML

- $\nabla_q \mathbb{H}(q) = \log q + 1$
- Functional *F*(*y*): an operator that takes a function *y*(*x*) and returns an output value *F*
- Functional derivative (aka, variational derivative) relates a change in a Functional F(y) to a change in the function y

- Recall the conventional derivative $\frac{dy}{dx}$
 - Taylor expansion

$$y(x + \epsilon) = y(x) + \frac{\mathrm{d}y}{\mathrm{d}x}\epsilon + O(\epsilon^2)$$

- Functional derivative
 - How much a functional F[y] changes when we make a small change $\varepsilon \eta(x)$ to the function y(x)

$$F[y(x) + \epsilon \eta(x)] = F[y(x)] + \epsilon \int \frac{\delta F}{\delta y(x)} \eta(x) \, \mathrm{d}x + O(\epsilon^2)$$

• A function y(x) that maximizes (or minimizes) a functional F[y] must satisfy δF

$$\frac{\partial I}{\partial y(x)} = 0$$
 for all x

$$F[y(x) + \epsilon \eta(x)] = F[y(x)] + \epsilon \int \frac{\delta F}{\delta y(x)} \eta(x) \, \mathrm{d}x + O(\epsilon^2)$$

- Consider a functional that is defined by an integral over a function G(y,x) $F[y] = \int G(y,x) dx$
- Consider variations in the function y(x),

$$F[y + \epsilon \eta(x)] = F[y(x)] + \epsilon \int \frac{\partial G}{\partial y} \eta(x) dx + O(\epsilon^2)$$

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- Ex.1, $-\mathbb{H}(q) = \int q(x) \log q(x) dx$ • $G = q(x) \log q(x)$
- EX.2, posterior regularization

Ex.2: Posterior Regularization

assume single $\min_{q,\xi} - H(q(z)) - \mathbb{E}_{q(z)} \left[\log p(x^*|z)\pi(z)\right] + \sum_i \xi_i$ data point x^*

s.t.
$$\mathbb{E}_q [T(\boldsymbol{x}^*, \boldsymbol{z})] \leq \boldsymbol{\xi}$$

 $\boldsymbol{\xi} \geq 0,$

• Lagrangian

 $\max_{\boldsymbol{\mu} \ge 0, \boldsymbol{\eta} \ge 0, \alpha \ge 0} \min_{q, \boldsymbol{\xi}} - H(q(\boldsymbol{z})) - \mathbb{E}_{q(\boldsymbol{z})} \left[\log p(\boldsymbol{x}^* | \boldsymbol{z}) \pi(\boldsymbol{z}) \right]$

$$+\sum_{i}(1-\mu_{i})\xi_{i}+\sum_{i}\eta_{i}\left(\mathbb{E}_{q}[T_{i}(\boldsymbol{x}^{*};\boldsymbol{z})]-\xi_{i}\right)+\alpha\left(\sum_{z}q(\boldsymbol{z})-1\right)$$

A "Standardized" View of ML

The general expression as a constrained optimization: (auxiliary) distribution q $\mathbf{x} = - \mathbf{x} \mathbf{x} \mathbf{x} \mathbf{x} \mathbf{x}$ $\mathbf{x} = - \mathbf{x} \mathbf{y} \mathbf{x} \mathbf{y}$

MaxEnt perspective

- Supervised MLE and maximum entropy
- Unsupervised MLE and maximum entropy
- Bayesian inference and maximum entropy
 - Bayesian inference as optimization
- Posterior regularization:
 - Constrained Bayesian inference => constrained optimization

s.t. $q \in Q$. so strained set

The general expression as a constrained optimization: (auxiliary) distribution q $q = q, \theta$ $f = q, \theta$

 $\min_{q(\boldsymbol{x},\boldsymbol{y})} H(q)$

s.t. $\mathbb{E}_q[T(\mathbf{x}, \mathbf{y})] = \mathbb{E}_{(\mathbf{x}^*, \mathbf{y}^*) \sim \mathcal{D}}[T(\mathbf{x}, \mathbf{y})]$

The general expression as a constrained optimization: (auxiliary) distribution q q, θ $f = --q, \theta$ $\mathcal{L}(q, \theta)$ $\mathcal{L}($

• Unsupervised MLE and maximum entropy

 $\min_{q,\theta} H(q(\boldsymbol{y}|\boldsymbol{x}^*)) + \mathbb{E}_{q(\boldsymbol{y}|\boldsymbol{x}^*)}[\log p_{\theta}(\boldsymbol{x}^*, \boldsymbol{y})]$

The general expression as a constrained optimization: (auxiliary) distribution q $q = q, \theta$ $f = q, \theta$

- Unsupervised MLE and maximum entropy
- Bayesian inference and maximum entropy

$$\min_{q(\boldsymbol{z})} - H(q(\boldsymbol{z})) + \log p(\mathcal{D}) - \mathbb{E}_{q(\boldsymbol{z})} \left[\log \pi(\boldsymbol{z}) + \sum_{\boldsymbol{x}^* \in \mathcal{D}} \log p(\boldsymbol{x}^* | \boldsymbol{z}) \right]$$

s.t. $q(\boldsymbol{z}) \in \mathcal{P}$

The general expression as a constrained optimization: (auxiliary) distribution q $\mathbf{x} = \frac{1}{\sqrt{q}} \int_{\mathbf{x}} \mathcal{L}(q, \theta)$

MaxEnt perspective

- Supervised MLE and maximum entropy
- Unsupervised MLE and maximum entropy
- Bayesian inference and maximum entropy
- Posterior regularization

$$\begin{split} \min_{q,\boldsymbol{\xi}} & -\mathrm{H}\left(q(\boldsymbol{z})\right) - \mathbb{E}_{q(\boldsymbol{z})}\left[\sum_{\boldsymbol{x}^* \in \mathcal{D}} \log p(\boldsymbol{x}^* | \boldsymbol{z}) \pi(\boldsymbol{z})\right] + U(\boldsymbol{\xi}) \\ & s.t. \ q(\boldsymbol{z}) \in \mathcal{Q}(\boldsymbol{\xi}) \\ & \boldsymbol{\xi} \geq 0, \end{split}$$

s.t. $q \in Q$. so strained set

- Let *t* be the variable of interest
 - E.g., the input-output pair t = (x, y) in a prediction task
 - or t = x in generative modeling
- $p_{\theta}(t)$: the target model to be learned
- q(t): auxiliary distribution
- The SE: $\min_{q,\theta,\xi} \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) + U(\xi)$ $s.t. \mathbb{E}_{q(t)}\left[f_{k}(t)\right] < \xi_{k}, \quad k = 1, ..., K$
 - $\circ~$ Experience function f~ represents external experiences of different kinds for training the model
 - $f_k(t) \in \mathbb{R}$: measures the goodness of a configuration t in light of any given experiences
 - Data, constraints, reward, adversarial discriminators, etc., can all be formulated as an experience function (later)
- Maximizing $\mathbb{E}_{q(t)}[f_k(t)] \rightarrow q$ is encouraged to produce samples receiving high scores [Hu & Xing, 2021]

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• The SE:
$$\min_{q,\theta,\xi} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) + U(\xi)$$
$$s.t. - \mathbb{E}_{q(t)}\left[f_{k}(t)\right] < \xi_{k}, \quad k = 1, \dots, K$$

- $\circ~$ Divergence D: measures the distance between the target model $~p_{\theta}$ to be trained and the auxiliary model q
 - E.g., cross entropy

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$$s.t. - \mathbb{E}_{q(t)}\left[f_{k}(t)\right] < \xi_{k}, \quad k = 1, \dots, K$$

- Uncertainty III: controls the compactness of the model
 - E.g., Shannon entropy

$$\min_{q, \theta, \xi} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) + U(\xi)$$

s.t. $-\mathbb{E}_{q(t)}\left[f_{k}(t)\right] < \xi_{k}, \quad k = 1, ..., K$

Assuming penalty
$$U = \sum_{k} \xi_{k}$$
, and $f = \sum_{k} f_{k}$:

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

3 terms:

Uncertainty (self-regularization) e.g., Shannon entropy



Divergence (fitness) e.g., Cross Entropy



Experiences

(exogenous regularizations) e.g., data examples, rules



$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

- The introduction of the auxiliary distribution q relaxes the learning problem of p_{θ} , originally only over θ , to be now alternating between q and θ
 - \circ Recall in EM, we introduced q to deal with the intractable marginal log-likelihood
- q acts as a conduit between the exogenous experience and the target model
 subsumes the experience, by maximizing the expected *f* value
 - \circ passes it incrementally to the target model, by minimizing the divergence \mathbb{D}
- E.g., assume \mathbb{D} is cross entropy, and \mathbb{H} is Shannon entropy
 - The above optimization, at each iteration *n*:

$$q^{(n+1)}(\boldsymbol{t}) = \exp\left\{\frac{\beta \log p_{\theta^{(n)}}(\boldsymbol{t}) + f(\boldsymbol{t})}{\alpha}\right\} / Z$$
$$\boldsymbol{\theta}^{(n+1)} = \operatorname*{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{q^{(n+1)}(\boldsymbol{t})} [\log p_{\theta}(\boldsymbol{t})],$$

19

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

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 - The above optimization, at each iteration n:

Teacher:
$$q^{(n+1)}(t) = \exp\left\{\frac{\beta \log p_{\theta^{(n)}}(t) + f(t)}{\alpha}\right\} / Z$$

Student:
$$\boldsymbol{\theta}^{(n+1)} = \operatorname*{argmax}_{\boldsymbol{\theta}} \mathbb{E}_{q^{(n+1)}(\boldsymbol{t})} [\log p_{\boldsymbol{\theta}}(\boldsymbol{t})],$$
 20

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

• Formulates a large space of learning algorithms, which encompasses many wellknown algorithms

SE encompasses many well-known algorithms (more later)

Experience type	Experience function f	Divergence \mathbb{D}	lpha	eta	Algorithm
Data instances	$f_{ ext{data}}(oldsymbol{x};\mathcal{D})$	CE	1	1	Unsupervised MLE
	$f_{ ext{data}}(oldsymbol{x},oldsymbol{y};\mathcal{D})$	CE	1	ϵ	Supervised MLE
	$f_{ ext{data-self}}(oldsymbol{x},oldsymbol{y};\mathcal{D})$	CE	1	ϵ	Self-supervised MLE
	$f_{ ext{data-w}}(oldsymbol{t};\mathcal{D})$	CE	1	ϵ	Data re-weighting
	$f_{ ext{data-aug}}(oldsymbol{t};\mathcal{D})$	CE	1	ϵ	Data Augmentation
	$f_{ ext{active}}(oldsymbol{x},oldsymbol{y};\mathcal{D})$	CE	1	ϵ	Active Learning (Ertekin et al., 2007)
Knowledge	$f_{rule}(oldsymbol{x},oldsymbol{y})$	CE	1	1	Posterior Regularization (Ganchev et al., 2010)
	$f_{rule}(oldsymbol{x},oldsymbol{y})$	CE	\mathbb{R}	1	Unified EM (Samdani et al., 2012)
Reward	$\log Q^{ heta}(oldsymbol{x},oldsymbol{y})$	CE	1	1	Policy Gradient
	$\log Q^{ heta}(oldsymbol{x},oldsymbol{y}) + Q^{in, heta}(oldsymbol{x},oldsymbol{y})$	CE	1	1	+ Intrinsic Reward
	$Q^{ heta}(oldsymbol{x},oldsymbol{y})$	CE	$\tau > 0$	$\tau > 0$	RL as Inference
Other advanced	binary classifier	JSD	0	1	Vanilla GAN (Goodfellow et al., 2014)
	discriminator	f-divg.	0	1	f-GAN (Nowozin et al., 2016)
	1-Lipschitz discriminator	W_1 dist.	0	1	WGAN (Arjovsky et al., 2017)
	1-Lipschitz discriminator	KL	0	1	PPO-GAN (Wu et al., 2020)

SE with supervised data experience

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

• Input-output variables t = (x, y)

- Experience: dataset $\mathcal{D} = \{(x^*, y^*)\}$ of size N
 - defines the empirical distribution

$$\widetilde{p}(\boldsymbol{x},\boldsymbol{y}) = \frac{m(\boldsymbol{x},\boldsymbol{y})}{N} = \mathbb{E}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)\sim\mathcal{D}}[\mathbb{1}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)}(\boldsymbol{x},\boldsymbol{y})]$$

The expected similarity between (x, y) and observed data (x^*, y^*) , with similarity measure $\mathbb{1}_a(b)$, i.e., an indicator function (1 if a=b, 0 otherwise)

SE with supervised data experience $\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$

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Define the experience function

$$f := f_{data}(\mathbf{x}, \mathbf{y}; \mathcal{D}) = \log \mathbb{E}_{(\mathbf{x}^*, \mathbf{y}^*) \sim \mathcal{D}} \left[\mathbb{1}_{(\mathbf{x}^*, \mathbf{y}^*)}(\mathbf{x}, \mathbf{y}) \right]$$

• Let \mathbb{D} cross entropy, \mathbb{H} Shannon entropy, $\alpha = 1, \beta = \epsilon$ (a very small value)

$$\min_{q,\theta} - H(q) - \epsilon \mathbb{E}_q \left[\log p_{\theta}(\boldsymbol{x}, \boldsymbol{y}) \right] - \mathbb{E}_q \left[f_{data}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) \right]$$

SE with supervised data experience

$$f := f_{data}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) = \log \mathbb{E}_{(\boldsymbol{x}^*, \boldsymbol{y}^*) \sim \mathcal{D}} \left[\mathbb{1}_{(\boldsymbol{x}^*, \boldsymbol{y}^*)}(\boldsymbol{x}, \boldsymbol{y}) \right]$$
$$\min_{q, \theta} - H(q) - \epsilon \mathbb{E}_q \left[\log p_{\theta}(\boldsymbol{x}, \boldsymbol{y}) \right] - \mathbb{E}_q \left[f_{data}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) \right]$$

• At each iteration *n*:

Teacher:
$$q^{(n+1)}(t) = \exp\left\{\frac{\beta \log p_{\theta^{(n)}}(t) + f(t)}{\alpha}\right\} / Z \approx \tilde{p}(\boldsymbol{x}, \boldsymbol{y})$$

Student: $\boldsymbol{\theta}^{(n+1)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \mathbb{E}_{q^{(n+1)}(t)}[\log p_{\theta}(t)],$
Maximizes data log-likelihood

Maximizes data log-likelihood

• Recovers supervised MLE!

SE with unsupervised data experience

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

• Input-output variables t = (x, y)

• Experience: dataset $\mathcal{D} = \{(x^*)\}$ of size N, I,e., we only observe the x part

• defines the empirical distribution

$$\widetilde{p}(\boldsymbol{x}) = \frac{m(\boldsymbol{x})}{N} = \mathbb{E}_{\boldsymbol{x}^* \sim \mathcal{D}}[\mathbb{1}_{\boldsymbol{x}^*}(\boldsymbol{x})]$$

• Define the experience function

$$f := f_{data}(\mathbf{x}; \mathcal{D}) = \log \mathbb{E}_{\mathbf{x}^* \sim \mathcal{D}}[\mathbb{1}_{\mathbf{x}^*}(\mathbf{x})]$$

• Let \mathbb{D} cross entropy, \mathbb{H} Shannon entropy, $\alpha = 1, \beta = 1$

$$\min_{q,\theta} - H(q) - \mathbb{E}_q \left[\log p_{\theta}(\boldsymbol{x}, \boldsymbol{y}) \right] - \mathbb{E}_q \left[f_{data}(\boldsymbol{x}; \mathcal{D}) \right]$$

• Assume $q(\mathbf{x}, \mathbf{y}) = \tilde{p}(\mathbf{x})q(\mathbf{y}|\mathbf{x})$

Recovers **unsupervised**

MLE (EM)!

SE with manipulated data experience

- Input-output variables t = (x, y)
- Experience: dataset $\mathcal{D} = \{(x^*, y^*)\}$ of size N
 - defines the empirical distribution

$$\tilde{p}(\boldsymbol{x},\boldsymbol{y}) = \frac{m(\boldsymbol{x},\boldsymbol{y})}{N} = \mathbb{E}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)\sim\mathcal{D}}[\mathbb{1}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)}(\boldsymbol{x},\boldsymbol{y})]$$

• Define the experience function

$$f := f_{data}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) = \log \mathbb{E}_{(\boldsymbol{x}^*, \boldsymbol{y}^*) \sim \mathcal{D}} \left[\mathbb{1}_{(\boldsymbol{x}^*, \boldsymbol{y}^*)}(\boldsymbol{x}, \boldsymbol{y}) \right]$$

- The similarity measure $\mathbb{1}_{a}(b)$ is too restrictive. Let's enrich it:
 - Don't have to be 0/1, we can scale it

 $f := f_{data-w}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) = \log \mathbb{E}_{(\boldsymbol{x}^*, \boldsymbol{y}^*) \sim \mathcal{D}} [w(\boldsymbol{x}^*, \boldsymbol{y}^*) \cdot \mathbb{1}_{(\boldsymbol{x}^*, \boldsymbol{y}^*)}(\boldsymbol{x}, \boldsymbol{y})]$

Plug *f_{data-w}* into SE, keep all other configurations the same as supervised MLE, we recover **data re-weighting** in the "student" step

$$\max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{t}^* \sim \mathcal{D}} \left[w(\boldsymbol{t}^*) \cdot \log p_{\boldsymbol{\theta}}(\boldsymbol{t}^*) \right]$$

SE with manipulated data experience

- Input-output variables t = (x, y)
- Experience: dataset $\mathcal{D} = \{(x^*, y^*)\}$ of size N
 - defines the empirical distribution

$$\tilde{p}(\boldsymbol{x},\boldsymbol{y}) = \frac{m(\boldsymbol{x},\boldsymbol{y})}{N} = \mathbb{E}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)\sim\mathcal{D}}[\mathbb{1}_{(\boldsymbol{x}^*,\boldsymbol{y}^*)}(\boldsymbol{x},\boldsymbol{y})]$$

• Define the experience function

$$f := f_{data}(\boldsymbol{x}, \boldsymbol{y}; \mathcal{D}) = \log \mathbb{E}_{(\boldsymbol{x}^*, \boldsymbol{y}^*) \sim \mathcal{D}} \left[\mathbb{1}_{(\boldsymbol{x}^*, \boldsymbol{y}^*)}(\boldsymbol{x}, \boldsymbol{y}) \right]$$

- The similarity measure $\mathbb{1}_{a}(b)$ is too restrictive. Let's enrich it:
 - Don't have to match exactly, we can relax it

$$f := f_{data-aug}(\mathbf{x}, \mathbf{y}; \mathcal{D}) = \log \mathbb{E}_{(\mathbf{x}^*, \mathbf{y}^*) \sim \mathcal{D}} \left[a_{(\mathbf{x}^*, \mathbf{y}^*)}(\mathbf{x}, \mathbf{y}) \right]$$

- a_(x*,y*)(x, y): assigns non-zero probability to not only the exact (x*, y*) but also other (x, y) configurations
- Plug $f_{data-aug}$ into SE, keep all other configurations the same as supervised MLE, we recover **data augmentation** in the "student" step $\max_{\theta} \mathbb{E}_{t^* \sim \mathcal{D}, t \sim a_{t^*}(t)} [\log p_{\theta}(t)]$.

SE with actively supervised experience

- Have access to a vast pool of unlabeled data instances
- Can select instances (queries) to be labeled by an oracle (e.g., human)
- Experiences:
 - $\circ u(x)$ measures informativeness of an instance x
 - e.g., Uncertainty on x, measured by predictive entropy
 - Instances + oracle labels:

$$f(\mathbf{x}, \mathbf{y}; Oracle) = \log \mathbb{E}_{x^* \sim \mathcal{D}, y^* \sim Oracle(x^*)} \left[\mathbb{1}_{(x^*, y^*)}(\mathbf{x}, \mathbf{y}) \right]$$

SE with actively supervised experience

$$\min_{q,\theta} - \alpha H(q) - \beta \mathbb{E}_q \left[\log p_{\theta}(\boldsymbol{x}, \boldsymbol{y}) \right] - \mathbb{E}_{q(\boldsymbol{x}, \boldsymbol{y})} \left[f(\boldsymbol{x}, \boldsymbol{y}) \right]$$

$$f \coloneqq f(\mathbf{x}, \mathbf{y}; Oracle) + u(\mathbf{x}) \qquad \alpha = 1, \beta = \epsilon$$

$$\downarrow$$
Teacher $q(\mathbf{x}, \mathbf{y}) = \exp\left\{\frac{\beta \log p_{\theta}(\mathbf{x}, \mathbf{y}) + f(\mathbf{x}, \mathbf{y}; Oracle) + u(\mathbf{x})}{\alpha}\right\} / Z$

• Student
$$\min_{\theta} - \mathbb{E}_q \left[\log p_{\theta}(\mathbf{x}, \mathbf{y}) \right]$$

 \bigcirc

Equivalent to **active learning** [e.g., Ertekin et al., 07]:

- Randomly draw a subset $\mathcal{D}_{sub} = \{x^*\}$
- Draw a query \mathbf{x}^* from \mathcal{D}_{sub} according to $\exp\{u(\mathbf{x})\}$
- Get label y* for x* from the oracle
- Maximize log likelihood on (x^*, y^*)

Key Takeaways

- (auxiliary) distribution $q \min_{q,\theta} \mathcal{L}(q,\theta)$ constrained set $s.t. \ q \in Q$. The MaxEnt perspective converts learning into a constrained optimization problem
- The standard equation (SE):

$$\min_{q,\theta} - \alpha \mathbb{H}(q) + \beta \mathbb{D}\left(q(t), p_{\theta}(t)\right) - \mathbb{E}_{q(t)}\left[f(t)\right]$$

3 terms:



Functional derivative

$$F[y(x) + \epsilon \eta(x)] = F[y(x)] + \epsilon \int \frac{\delta F}{\delta y(x)} \eta(x) \, \mathrm{d}x + O(\epsilon^2)$$

31

Questions?