Foundations of Machine Learning

Maximum Entropy Models, Logistic Regression

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Motivation

- Probabilistic models:
  - density estimation.
  - classification.

This Lecture

- Notions of information theory.
- Introduction to density estimation.
- Maxent models.
- Conditional Maxent models.

Entropy

(Shannon, 1948)

- Definition: the entropy of a discrete random variable X with probability mass distribution $\mathsf{p}(x) = \Pr[X = x]$ is

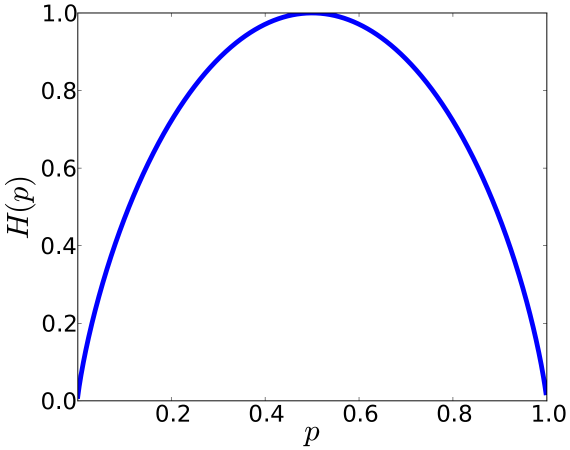
$$H(X) = -\mathrm{E}[\log \mathsf{p}(X)] = -\sum_{x \in X} \mathsf{p}(x) \log \mathsf{p}(x).$$

- Properties:
  - $H(X) \geq 0.$
  - measure of uncertainty of X.
  - maximal for uniform distribution. For a finite support, by Jensen's inequality:

$$H(X) = \mathrm{E}\left[\log \frac{1}{\mathsf{p}(X)}\right] \leq \log \mathrm{E}\left[\frac{1}{\mathsf{p}(X)}\right] = \log N.$$

Entropy

- Base of logarithm: not critical; for base 2, $-\log_2(\mathsf{p}(x))$ is the number of bits needed to represent $\mathsf{p}(x)$.
- Definition and notation: the entropy of a distribution p is defined by the same quantity and denoted by $H(\mathsf{p})$.
- Special case of Rényi entropy (Rényi, 1961).
- Binary entropy: $H(\mathsf{p}) = -\mathsf{p}\log\mathsf{p} - (1-\mathsf{p})\log(1-\mathsf{p})$.



Relative Entropy

(Shannon, 1948; Kullback and Leibler, 1951)

- Definition: the relative entropy (or Kullback-Leibler divergence) between two distributions p and q (discrete case) is

$$D(\mathsf{p} \,\|\, \mathsf{q}) = \mathrm{E}_{\mathsf{p}}\left[\log \frac{\mathsf{p}(X)}{\mathsf{q}(X)}\right] = \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \frac{\mathsf{p}(x)}{\mathsf{q}(x)},$$

with $0 \log \frac{0}{\mathsf{q}} = 0 \text{ and } \mathsf{p} \log \frac{\mathsf{p}}{0} = +\infty.$

- Properties:
  - asymmetric: in general, $D(\mathsf{p} \,\|\, \mathsf{q}) \neq D(\mathsf{q} \,\|\, \mathsf{p})$ for $\mathsf{p} \neq \mathsf{q}$.
  - non-negative: $D(\mathsf{p} \,\|\, \mathsf{q}) \geq 0$ for all p and q.
  - definite: $(D(\mathsf{p} \,\|\, \mathsf{q}) = 0) \Rightarrow (\mathsf{p} = \mathsf{q})$.

Non-Negativity of Rel. Entropy

- By the concavity of log and Jensen's inequality,

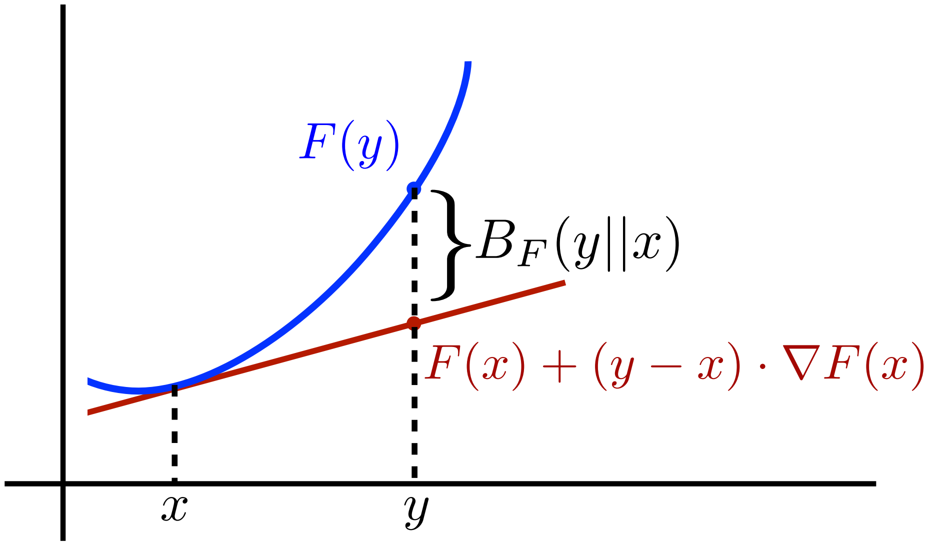
$$\begin{aligned}
-D(\mathsf{p} \parallel \mathsf{q}) &= \sum_{x\colon\, \mathsf{p}(x)>0} \mathsf{p}(x) \log\left(\frac{\mathsf{q}(x)}{\mathsf{p}(x)}\right) \\
&\leq \log\left(\sum_{x\colon\, \mathsf{p}(x)>0} \mathsf{p}(x)\frac{\mathsf{q}(x)}{\mathsf{p}(x)}\right) \\
&= \log\left(\sum_{x\colon\, \mathsf{p}(x)>0} \mathsf{q}(x)\right) \leq \log(1) = 0.
\end{aligned}$$

Bregman Divergence

(Bregman, 1967)

- Definition: let F be a convex and differentiable function defined over a convex set C in a Hilbert space $\mathbb{H}$. Then, the Bregman divergence B_F associated to F is defined by

$$B_F(x \parallel y) = F(x) - F(y) - \langle \nabla F(y), x - y \rangle \, .$$



Bregman Divergence

- Examples:

	$\boldsymbol{B_F(x \parallel y)}$	$\boldsymbol{F(x)}$
Squared L_2-distance	$\lVert\mathbf{x}-\mathbf{y}\rVert^2$	$\lVert\mathbf{x}\rVert^2$
Mahalanobis distance	$(\mathbf{x}-\mathbf{y})^\top\mathbf{K}^{-1}(\mathbf{x}-\mathbf{y})$	$\mathbf{x}^\top\mathbf{K}^{-1}\mathbf{x}$
Unnormalized relative entropy	$\widetilde{D}(\mathbf{x} \parallel \mathbf{y})$	$\sum_{i\in I} x_i \log x_i - x_i$

  - note: relative entropy not a Bregman divergence since not defined over an open set; but, on the simplex, coincides with unnormalized relative entropy

$$\widetilde{D}(\mathsf{p} \parallel \mathsf{q}) = \sum_{x\in\mathcal{X}} \mathsf{p}(x) \log\left[\frac{\mathsf{p}(x)}{\mathsf{q}(x)}\right] + \big(\mathsf{q}(x) - \mathsf{p}(x)\big).$$

Conditional Relative Entropy

- Definition: let p and q be two probability distributions over $\mathcal{X} \times \mathcal{Y}$. Then, the conditional relative entropy of p and q with respect to distribution r over $\mathcal{X}$ is defined by

$$\begin{aligned}\operatorname*{E}_{X \sim \mathsf{r}}\Big[D\big(\mathsf{p}(\cdot|X) \parallel \mathsf{q}(\cdot|X)\big)\Big] &= \sum_{x \in \mathcal{X}} \mathsf{r}(x) \sum_{y \in \mathcal{Y}} \mathsf{p}(y|x) \log \frac{\mathsf{p}(y|x)}{\mathsf{q}(y|x)} \\ &= D(\widetilde{\mathsf{p}} \parallel \widetilde{\mathsf{q}}),\end{aligned}$$

  with $\widetilde{\mathsf{p}}(x, y) = \mathsf{r}(x)\mathsf{p}(y|x)$, $\widetilde{\mathsf{q}}(x, y) = \mathsf{r}(x)\mathsf{q}(y|x)$, and the conventions $0 \log 0 = 0$, $0 \log \frac{0}{0} = 0$, and $\mathsf{p} \log \frac{\mathsf{p}}{0} = +\infty$.

  - note: the definition of conditional relative entropy is not intrinsic, it depends on a third distribution r.

This Lecture

- Notions of information theory.
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Density Estimation Problem

- Training data: sample S of size m drawn i.i.d. from set $\mathcal{X}$ according to some distribution $\mathcal{D}$,

$$S = (x_1, \ldots, x_m).$$

- Problem: find distribution p out of hypothesis set $\mathcal{P}$ that best estimates $\mathcal{D}$.

Maximum Likelihood Solution

- Maximum Likelihood principle: select distribution $\mathsf{p} \in \mathcal{P}$ maximizing likelihood of observed sample S,

$$\begin{aligned} \mathsf{p}_{\mathrm{ML}} &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \Pr[S|\mathsf{p}] \\ &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \prod_{i=1}^{m} \mathsf{p}(x_i) \\ &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \sum_{i=1}^{m} \log \mathsf{p}(x_i). \end{aligned}$$

Relative Entropy Formulation

- Lemma: let $\widehat{\mathsf{p}}_S$ be the empirical distribution for sample S, then

$$\mathsf{p}_{\mathrm{ML}} = \underset{\mathsf{p} \in \mathcal{P}}{\operatorname{argmin}}\, D(\widehat{\mathsf{p}}_S \parallel \mathsf{p}).$$

- Proof:

$$\begin{aligned} D(\widehat{\mathsf{p}}_S \parallel \mathsf{p}) &= \sum_x \widehat{\mathsf{p}}_S(x) \log \widehat{\mathsf{p}}_S(x) - \sum_x \widehat{\mathsf{p}}_S(x) \log \mathsf{p}(x) \\ &= -H(\widehat{\mathsf{p}}_S) - \sum_x \frac{\sum_{i=1}^m 1_{x=x_i}}{m} \log \mathsf{p}(x) \\ &= -H(\widehat{\mathsf{p}}_S) - \sum_{i=1}^m \sum_x \frac{1_{x=x_i}}{m} \log \mathsf{p}(x) \\ &= -H(\widehat{\mathsf{p}}_S) - \sum_{i=1}^m \frac{\log \mathsf{p}(x_i)}{m}. \end{aligned}$$

Maximum a Posteriori (MAP)

- Maximum a Posteriori principle: select distribution $\mathsf{p} \in \mathcal{P}$ that is the most likely, given the observed sample S and assuming a prior distribution $\Pr[\mathsf{p}]$ over $\mathcal{P}$,

$$\begin{aligned} \mathsf{p}_{\text{MAP}} &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \Pr[\mathsf{p}|S] \\ &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \frac{\Pr[S|\mathsf{p}] \Pr[\mathsf{p}]}{\Pr[S]} \\ &= \operatorname*{argmax}_{\mathsf{p} \in \mathcal{P}} \Pr[S|\mathsf{p}] \Pr[\mathsf{p}]. \end{aligned}$$

  - note: for a uniform prior, ML = MAP.

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Density Estimation + Features

- Training data: sample S of size m drawn i.i.d. from set $\mathcal{X}$ according to some distribution $\mathcal{D}$,

$$S = (x_1, \ldots, x_m).$$

- Features: associated to elements of $\mathcal{X}$,

$$\begin{aligned} \mathbf{\Phi} \colon \mathcal{X} &\to \mathbb{R}^N \\ x &\mapsto \mathbf{\Phi}(x) = \begin{bmatrix} \Phi_1(x) \\ \vdots \\ \Phi_N(x) \end{bmatrix}. \end{aligned}$$

- Problem: find distribution p out of hypothesis set $\mathcal{P}$ that best estimates $\mathcal{D}$.
  - for simplicity, in what follows, $\mathcal{X}$ is assumed to be finite.

Features

- Feature functions Φ_j assumed to be in H and $\|\mathbf{\Phi}\|_\infty \leq \Lambda$.
- Examples of H:
  - family of threshold functions $\{\mathbf{x} \mapsto 1_{x_i \leq \theta} \colon \mathbf{x} \in \mathbb{R}^N, \theta \in \mathbb{R}\}$ defined over N variables.
  - functions defined via decision trees with larger depths.
  - k-degree monomials of the original features.
  - zero-one features (often used in NLP, e.g., presence/ absence of a word or POS tag).

Maximum Entropy Principle

(E. T. Jaynes, 1957, 1983)

- Idea: empirical feature vector average close to expectation. For any $\delta > 0$, with probability at least $1 - \delta$

$$\left\| \underset{x\sim\mathcal{D}}{\mathrm{E}}[\mathbf{\Phi}(x)] - \underset{x\sim\widehat{\mathcal{D}}}{\mathrm{E}}[\mathbf{\Phi}(x)] \right\|_\infty \leq 2\mathfrak{R}_m(H) + \Lambda\sqrt{\frac{\log\frac{2}{\delta}}{2m}},$$

- Maxent principle: find distribution p that is closest to a prior distribution p_0 (typically uniform distribution) while verifying $\left\| \mathrm{E}_{x\sim\mathsf{p}}[\mathbf{\Phi}(x)] - \mathrm{E}_{x\sim\widehat{\mathcal{D}}}[\mathbf{\Phi}(x)] \right\|_\infty \leq \beta$.
- Closeness is measured using relative entropy.
  - note: no set $\mathcal{P}$ needed to be specified.

Maxent Formulation

- Optimization problem:

$$\min_{\mathsf{p}\in\Delta} D(\mathsf{p} \parallel \mathsf{p}_0)$$

$$\text{subject to: } \left\| \mathop{\mathrm{E}}_{x\sim\mathsf{p}}[\mathbf{\Phi}(x)] - \mathop{\mathrm{E}}_{x\sim S}[\mathbf{\Phi}(x)] \right\|_\infty \leq \beta.$$

  - convex optimization problem, unique solution.
  - $\beta = 0$: standard Maxent (or unregularized Maxent).
  - $\beta > 0$: regularized Maxent.

Relation with Entropy

- Relationship with entropy: for a uniform prior p_0,

$$\begin{aligned} D(\mathsf{p} \parallel \mathsf{p}_0) &= \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \frac{\mathsf{p}(x)}{\mathsf{p}_0(x)} \\ &= -\sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}_0(x) + \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}(x) \\ &= \log |\mathcal{X}| - H(\mathsf{p}). \end{aligned}$$

Maxent Problem

- Optimization: convex optimization problem.

$$\begin{aligned} \min_{\mathsf{p}} \quad & \sum_{x \in \mathcal{X}} \mathsf{p}(x) \log \mathsf{p}(x) \\ \text{subject to: } & \mathsf{p}(x) \geq 0, \forall x \in \mathcal{X} \\ & \sum_{x \in \mathcal{X}} \mathsf{p}(x) = 1 \\ & \left| \sum_{x \in \mathcal{X}} \mathsf{p}(x) \Phi_j(x) - \frac{1}{m} \sum_{i=1}^{m} \Phi_j(x_i) \right| \leq \beta, \forall j \in [1, N]. \end{aligned}$$

Gibbs Distributions

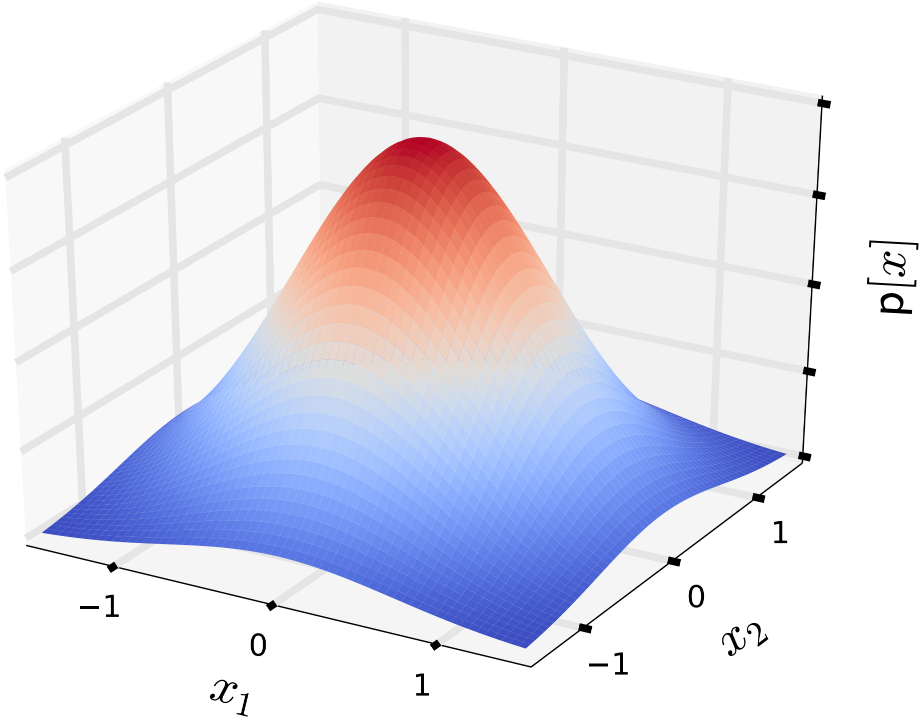
- Gibbs distributions: set $\mathcal{Q}$ of distributions $p_{\mathbf{w}}$ with $\mathbf{w} \in \mathbb{R}^N$,

$$\mathsf{p}_{\mathbf{w}}[x] = \frac{\mathsf{p}_0[x] \exp\big(\mathbf{w} \cdot \boldsymbol{\Phi}(x)\big)}{Z} = \frac{\mathsf{p}_0[x] \exp\big(\sum_{j=1}^N w_j \Phi_j(x)\big)}{Z},$$

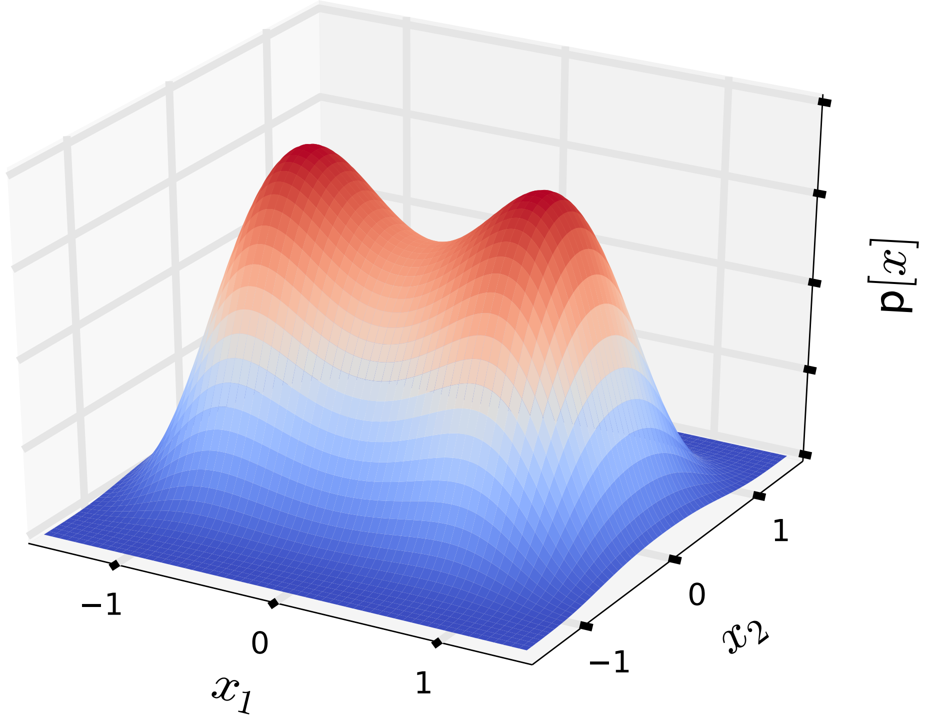
with $Z = \sum_x \mathsf{p}_0[x] \exp\big(\mathbf{w} \cdot \boldsymbol{\Phi}(x)\big)$.

- Rich family:
  - for linear and quadratic features: includes Gaussians and other distributions with non-PSD quadratic forms in exponents.
  - for higher-degree polynomials of raw features: more complex multi-modal distributions.

Examples



$$\mathsf{p}[(x_1, x_2)] = \frac{e^{-(x_1^2+x_2^2)}}{Z}.$$



$$\mathsf{p}[(x_1, x_2)] = \frac{e^{-(x_1^4+x_2^4)+x_1^2-x_2^2}}{Z}.$$

Dual Problems

- Regularized Maxent problem:

$$\min_{\mathsf{p}} F(\mathsf{p}) = \overline{D}(\mathsf{p} \parallel \mathsf{p}_0) + I_C(\operatorname*{E}_{\mathsf{p}}[\mathbf{\Phi}]),$$

$$\text{with } \begin{cases} \overline{D}(\mathsf{p} \parallel \mathsf{p}_0) = D(\mathsf{p} \parallel \mathsf{p}_0) \text{ if } \mathsf{p} \in \Delta\text{, } +\infty \text{ otherwise;} \\ C = \left\{\mathbf{u} \colon \|\mathbf{u} - \operatorname*{E}_{S}[\mathbf{\Phi}]\,\|_\infty \leq \beta\right\}; \\ I_C(x) = 0 \text{ if } x \in C\text{, } I_C(x) = +\infty \text{ otherwise.} \end{cases}$$

- Regularized Maximum Likelihood problem with Gibbs distributions:

$$\sup_{\mathbf{w}} G(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} \log \left[\frac{\mathsf{p}_{\mathbf{w}}[x_i]}{\mathsf{p}_0[x_i]}\right] - \beta \|\mathbf{w}\|_1.$$

Duality Theorem

(Della Pietra et al., 1997; Dudík et al., 2007; Cortes et al., 2015)

- Theorem: the regularized Maxent and ML with Gibbs distributions problems are equivalent,

$$\sup_{\mathbf{w} \in \mathbb{R}^N} G(\mathbf{w}) = \min_{\mathsf{p}} F(\mathsf{p}).$$

  - furthemore, let $\mathsf{p}^* = \operatorname*{argmin}_{\mathsf{p}} F(\mathsf{p})$, then, for any $\epsilon > 0$,

$$\left(\left| G(\mathbf{w}) - \sup_{\mathbf{w} \in \mathbb{R}^N} G(\mathbf{w}) \right| < \epsilon \right) \Rightarrow \Big(D(\mathsf{p}^* \parallel \mathsf{p}_{\mathbf{w}}) \leq \epsilon \Big).$$

Notes

- Maxent formulation:
  - no explicit restriction to a family of distributions $\mathcal{P}$.
  - but solution coincides with regularized ML with a specific family $\mathcal{P}$!
  - more general Bregman divergence-based formulation.

L_1-Regularized Maxent

(Kazama and Tsujii, 2003)

- Optimization problem:

$$\inf_{\mathbf{w}\in\mathbb{R}^N} \beta\|\mathbf{w}\|_1 - \frac{1}{m}\sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[x_i].$$

$$\text{where } \mathsf{p}_{\mathbf{w}}[x] = \frac{1}{Z}\exp\big(\mathbf{w}\cdot\mathbf{\Phi}(x)\big).$$

- Bayesian interpretation: equivalent to MAP with Laplacian prior $q_{\text{prior}}(\mathbf{w})$ (Williams, 1994),

$$\max_{\mathbf{w}} \log\Big(\prod_{i=1}^{m} \mathsf{p}_{\mathbf{w}}[x_i]\, \mathsf{q}_{\text{prior}}(\mathbf{w})\Big)$$

$$\text{with } q_{\text{prior}}(\mathbf{w}) = \prod_{j=1}^{N} \frac{\beta_j}{2}\exp(-\beta_j|w_j|).$$

Generalization Guarantee

(Dudík et al., 2007)

- Notation: $\mathcal{L}_{\mathcal{D}}(\mathbf{w}) = \mathop{\mathrm{E}}_{x \sim \mathcal{D}}[-\log \mathsf{p}_{\mathbf{w}}[x]]$, $\mathcal{L}_S(\mathbf{w}) = \mathop{\mathrm{E}}_{x \sim S}[-\log \mathsf{p}_{\mathbf{w}}[x]]$.
- Theorem: Fix $\delta > 0$. Let $\widehat{\mathbf{w}}$ be the solution of the L1-reg. Maxent problem for $\beta = 2\mathfrak{R}_m(H) + \Lambda\sqrt{\log(\frac{2}{\delta})/2m}$. Then, with probability at least $1 - \delta$,

$$\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) \leq \inf_{\mathbf{w}} \mathcal{L}_{\mathcal{D}}(\mathbf{w}) + 2\|\mathbf{w}\|_1 \left[2\mathfrak{R}_m(H) + \Lambda\sqrt{\frac{\log \frac{2}{\delta}}{2m}}\right].$$

Proof

- By Hölder's inequality and the concentration bound for average feature vectors,

$$\begin{aligned}\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_S(\widehat{\mathbf{w}}) &= \widehat{\mathbf{w}} \cdot \big[\mathop{\mathrm{E}}_{S}[\mathbf{\Phi}] - \mathop{\mathrm{E}}_{\mathcal{D}}[\mathbf{\Phi}]\big] \\ &\leq \|\widehat{\mathbf{w}}\|_1 \, \|\mathop{\mathrm{E}}_{S}[\mathbf{\Phi}] - \mathop{\mathrm{E}}_{\mathcal{D}}[\mathbf{\Phi}]\|_\infty \leq \beta \|\widehat{\mathbf{w}}\|_1.\end{aligned}$$

- Since $\widehat{\mathbf{w}}$ is a minimizer,

$$\begin{aligned}\mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) &= \mathcal{L}_{\mathcal{D}}(\widehat{\mathbf{w}}) - \mathcal{L}_S(\widehat{\mathbf{w}}) + \mathcal{L}_S(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \\ &\leq \beta \|\widehat{\mathbf{w}}\|_1 + \mathcal{L}_S(\widehat{\mathbf{w}}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \\ &\leq \beta \|\mathbf{w}\|_1 + \mathcal{L}_S(\mathbf{w}) - \mathcal{L}_{\mathcal{D}}(\mathbf{w}) \leq 2\beta \|\mathbf{w}\|_1. \\ &\qquad (\widehat{\mathbf{w}} \text{ minimizer of } \beta\|\mathbf{w}\|_1 + \mathcal{L}_S(\mathbf{w}))\end{aligned}$$

L_2-Regularized Maxent

(Chen and Rosenfeld, 2000; Lebanon and Lafferty, 2001)

- Different relaxations:
  - L_1 constraints:

$$\forall j \in [1, N], \quad \left| \mathop{\mathrm{E}}_{x \sim p}[\Phi_j(x)] - \mathop{\mathrm{E}}_{x \sim \widehat{p}}[\Phi_j(x)] \right| \leq \beta_j.$$

  - L_2 constraints:

$$\left\| \mathop{\mathrm{E}}_{x \sim p}[\mathbf{\Phi}(x)] - \mathop{\mathrm{E}}_{x \sim \widehat{p}}[\mathbf{\Phi}(x)] \right\|_2 \leq B.$$

L_2-Regularized Maxent

- Optimization problem:

$$\inf_{\mathbf{w} \in \mathbb{R}^N} \beta \|\mathbf{w}\|_2^2 - \frac{1}{m} \sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[x_i].$$

$$\text{where } \mathsf{p}_{\mathbf{w}}[x] = \frac{1}{Z} \exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x)\big).$$

- Bayesian interpretation: equivalent to MAP with Gaussian prior $q_{\text{prior}}(\mathbf{w})$ (Goodman, 2004),

$$\max_{\mathbf{w}} \ \log\Big(\prod_{i=1}^{m} \mathsf{p}_{\mathbf{w}}[x_i]\, \mathsf{q}_{\text{prior}}(\mathbf{w})\Big)$$

$$\text{with } \mathsf{q}_{\text{prior}}(\mathbf{w}) = \prod_{j=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{w_j^2}{2\sigma^2}}.$$

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Conditional Maxent Models

- Maxent models for conditional probabilities:
  - conditional probability modeling each class.
  - use in multi-class classification.
  - can use different features for each class.
  - a.k.a. multinomial logistic regression.
  - logistic regression: special case of two classes.

Problem

- Data: sample drawn i.i.d. according to some distribution D,

$$S = ((x_1, y_1), \ldots, (x_m, y_m)) \in (\mathcal{X} \times \mathcal{Y})^m.$$

  - $\mathcal{Y} = \{1, \ldots, k\}$, or $\mathcal{Y} = \{0, 1\}^k$ in multi-label case.

- Features: mapping $\mathbf{\Phi} \colon \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^N$.

- Problem: find accurate conditional probability models $\Pr[\cdot \mid x]$, $x \in \mathcal{X}$, based on $\mathbf{\Phi}$.

Conditional Maxent Principle

(Berger et al., 1996; Cortes et al., 2015)

- Idea: empirical feature vector average close to expectation. For any $\delta > 0$, with probability at least $1 - \delta$,

$$\left\| \underset{\substack{x\sim\widehat{\mathsf{p}}\\ y\sim\mathcal{D}[\cdot|x]}}{\mathrm{E}}[\boldsymbol{\Phi}(x,y)] - \underset{\substack{x\sim\widehat{\mathsf{p}}\\ y\sim\widehat{\mathsf{p}}[\cdot|x]}}{\mathrm{E}}[\boldsymbol{\Phi}(x,y)] \right\|_\infty \leq 2\mathfrak{R}_m(H) + \sqrt{\frac{\log\frac{2}{\delta}}{2m}}.$$

- Maxent principle: find conditional distributions $\mathsf{p}[\cdot|x]$ that are closest to priors $\mathsf{p}_0[\cdot|x]$ (typically uniform distributions) while verifying $\left\| \mathrm{E}_{\substack{x\sim\widehat{\mathsf{p}}\\ y\sim\mathsf{p}[\cdot|x]}}[\boldsymbol{\Phi}(x,y)] - \mathrm{E}_{\substack{x\sim\widehat{\mathsf{p}}\\ y\sim\widehat{\mathsf{p}}[\cdot|x]}}[\boldsymbol{\Phi}(x,y)] \right\|_\infty \leq \beta$.

- Closeness is measured using conditional relative entropy based on $\widehat{\mathsf{p}}$.

Cond. Maxent Formulation

(Berger et al., 1996; Cortes et al., 2015)

- Optimization problem: find distribution p solution of

$$\min_{\mathsf{p}[\cdot|x] \in \Delta} \sum_{x \in \mathcal{X}} \widehat{\mathsf{p}}[x] \, D\big(\mathsf{p}[\cdot|x] \parallel \mathsf{p}_0[\cdot|x]\big)$$

$$\text{s.t.} \; \left\| \mathop{\mathrm{E}}_{x \sim \widehat{\mathsf{p}}} \left[\mathop{\mathrm{E}}_{y \sim \mathsf{p}[\cdot|x]} [\mathbf{\Phi}(x, y)] \right] - \mathop{\mathrm{E}}_{(x,y) \sim S} [\mathbf{\Phi}(x, y)] \right\|_\infty \leq \beta.$$

  - convex optimization problem, unique solution.
  - $\beta = 0$: unregularized conditional Maxent.
  - $\beta > 0$: regularized conditional Maxent.

Dual Problems

- Regularized conditional Maxent problem:

$$\widetilde{F}(\mathsf{p}) = \mathop{\mathrm{E}}_{x\sim\widehat{p}}\left[\overline{D}\big(\mathsf{p}[\cdot|x] \parallel \mathsf{p}_0[\cdot|x]\big) + I_\Delta\big(\mathsf{p}[\cdot|x]\big)\right] + I_C\Big(\mathop{\mathrm{E}}_{\substack{x\sim\widehat{\mathsf{p}}\\ y\sim\mathsf{p}[\cdot|x]}}[\mathbf{\Phi}]\Big).$$

- Regularized Maximum Likelihood problem with conditional Gibbs distributions:

$$\widetilde{G}(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m}\log\left[\frac{\mathsf{p}_{\mathbf{w}}[y_i|x_i]}{\mathsf{p}_0[y_i|x_i]}\right] - \beta\|\mathbf{w}\|_1\,,$$

where $\forall(x,y)\in\mathcal{X}\times\mathcal{Y}$,

$$\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\mathsf{p}_0[y|x]\exp\big(\mathbf{w}\cdot\mathbf{\Phi}(x,y)\big)}{Z(x)}$$

$$Z(x) = \sum_{y\in\mathcal{Y}}\mathsf{p}_0[y|x]\exp(\mathbf{w}\cdot\mathbf{\Phi}(x,y)).$$

Duality Theorem

(Cortes et al., 2015)

- Theorem: the regularized conditional Maxent and ML with conditional Gibbs distributions problems are equivalent,

$$\sup_{\mathbf{w}\in\mathbb{R}^N} \widetilde{G}(\mathbf{w}) = \min_{\mathsf{p}} \widetilde{F}(\mathsf{p}).$$

  - furthemore, let $\mathsf{p}^* = \operatorname*{argmin}_{\mathsf{p}} \widetilde{F}(\mathsf{p})$, then, for any $\epsilon > 0$,

$$\Big(|\widetilde{G}(\mathbf{w}) - \sup_{\mathbf{w}\in\mathbb{R}^N} \widetilde{G}(\mathbf{w})| < \epsilon\Big) \Rightarrow \mathop{\mathrm{E}}_{x\sim\widehat{p}}\Big[D\big(\mathsf{p}^*[\cdot|x] \parallel \mathsf{p}_{\mathbf{w}}[\cdot|x]\big)\Big] \leq \epsilon.$$

Regularized Cond. Maxent

(Berger et al., 1996; Cortes et al., 2015)

- Optimization problem: convex optimizations, regularization parameter $\lambda \geq 0$.

$$\min_{\mathbf{w} \in \mathbb{R}^N} \lambda \|\mathbf{w}\|_1 - \frac{1}{m} \sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[y_i | x_i]$$

$$\text{or} \quad \min_{\mathbf{w} \in \mathbb{R}^N} \lambda \|\mathbf{w}\|_2^2 - \frac{1}{m} \sum_{i=1}^{m} \log \mathsf{p}_{\mathbf{w}}[y_i | x_i],$$

where $\forall (x, y) \in \mathcal{X} \times \mathcal{Y},$

$$\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x, y)\big)}{Z(x)}$$

$$Z(x) = \sum_{y \in \mathcal{Y}} \exp\big(\mathbf{w} \cdot \mathbf{\Phi}(x, y)\big).$$

More Explicit Forms

- Optimization problem: multinomial logistic loss.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} + \frac{1}{m}\sum_{i=1}^{m} \log\left[\sum_{y\in\mathcal{Y}} \exp\Big(\mathbf{w}\cdot\mathbf{\Phi}(x_i, y) - \mathbf{w}\cdot\mathbf{\Phi}(x_i, y_i)\Big)\right].$$

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} - \mathbf{w}\cdot\frac{1}{m}\sum_{i=1}^{m}\mathbf{\Phi}(x_i, y_i) + \frac{1}{m}\sum_{i=1}^{m}\log\left[\sum_{y\in\mathcal{Y}} e^{\mathbf{w}\cdot\mathbf{\Phi}(x_i, y)}\right].$$

Related Problem

- Optimization problem: log-sum-exp replaced by max.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} + \frac{1}{m}\sum_{i=1}^{m} \underbrace{\max_{y\in\mathcal{Y}}\Big(\mathbf{w}\cdot\mathbf{\Phi}(x_i,y) - \mathbf{w}\cdot\mathbf{\Phi}(x_i,y_i)\Big)}_{-\rho_{\mathbf{w}}(x_i,y_i)}.$$

Common Feature Choice

- Multi-class features:

$$\mathbf{\Phi}(x,y) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \mathbf{\Gamma}(x) \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} \mathbf{w}_1 \\ \vdots \\ \mathbf{w}_{y-1} \\ \mathbf{w}_y \\ \mathbf{w}_{y+1} \\ \vdots \\ \mathbf{w}_{|\mathcal{Y}|} \end{bmatrix} \quad \longrightarrow \quad \mathbf{w} \cdot \mathbf{\Phi}(x,y) = \mathbf{w}_y \cdot \mathbf{\Gamma}(x).$$

- L2-regularized cond. maxent optimization:

$$\min_{\mathbf{w} \in \mathbb{R}^N} \lambda \sum_{y \in \mathcal{Y}} \|\mathbf{w}_y\|_2^2 + \frac{1}{m} \sum_{i=1}^{m} \log \left[\sum_{y \in \mathcal{Y}} \exp \Big(\mathbf{w}_y \cdot \mathbf{\Gamma}(x_i) - \mathbf{w}_{y_i} \cdot \mathbf{\Gamma}(x_i) \Big) \right].$$

Prediction

- Prediction with $\mathsf{p}_{\mathbf{w}}[y|x] = \frac{\exp(\mathbf{w}\cdot\mathbf{\Phi}(x,y))}{Z(x)}$:

$$\widehat{y}(x) = \text{argmax}_{y\in\mathcal{Y}}\ \mathsf{p}_{\mathbf{w}}[y|x] = \text{argmax}_{y\in\mathcal{Y}}\ \mathbf{w}\cdot\mathbf{\Phi}(x,y).$$

Binary Classification

- Simpler expression:

$$\begin{aligned}
&\sum_{y\in\mathcal{Y}} \exp\Big(\mathbf{w}\cdot\mathbf{\Phi}(x_i, y) - \mathbf{w}\cdot\mathbf{\Phi}(x_i, y_i)\Big)\\
&= e^{\mathbf{w}\cdot\mathbf{\Phi}(x_i,+1)-\mathbf{w}\cdot\mathbf{\Phi}(x_i,y_i)} + e^{\mathbf{w}\cdot\mathbf{\Phi}(x_i,-1)-\mathbf{w}\cdot\mathbf{\Phi}(x_i,y_i)}\\
&= 1 + e^{-y_i\mathbf{w}\cdot[\mathbf{\Phi}(x_i,+1)-\mathbf{\Phi}(x_i,-1)]}\\
&= 1 + e^{-y_i\mathbf{w}\cdot\mathbf{\Psi}(x_i)},
\end{aligned}$$

with $\mathbf{\Psi}(x) = \mathbf{\Phi}(x, +1) - \mathbf{\Phi}(x, -1)$.

Logistic Regression

(Berkson, 1944)

- Binary case of conditional Maxent.
- Optimization problem: regularized logistic loss.

$$\min_{\mathbf{w}\in\mathbb{R}^N} \begin{cases} \lambda\|\mathbf{w}\|_1 \\ \lambda\|\mathbf{w}\|_2^2 \end{cases} + \frac{1}{m}\sum_{i=1}^{m} \log\left[1 + e^{-y_i \mathbf{w}\cdot\mathbf{\Psi}(x_i)}\right].$$

  - convex optimization.
  - variety of solutions: SGD, coordinate descent, etc.
  - coordinate descent: similar to AdaBoost with logistic loss $\phi(-u) = \log_2(1 + e^{-u}) \geq 1_{u\leq 0}$ instead of exponential loss.

Generalization Bound

- Theorem: assume that $\pm\Phi_j \in H$ for all $j \in [1, N]$. Then, for any $\delta > 0$, with probability at least $1-\delta$ over the draw of a sample S of size m, for all $f\colon x \mapsto \mathbf{w} \cdot \Phi(x)$,

$$R(f) \leq \frac{1}{m}\sum_{i=1}^{m} \log_{u_0}\Big(1 + e^{-y_i \mathbf{w}\cdot\Phi(x_i)}\Big) + 4\|\mathbf{w}\|_1 \mathfrak{R}_m(H)$$
$$+ \sqrt{\frac{\log\log_2 2\|\mathbf{w}\|_1}{m}} + \sqrt{\frac{\log\frac{2}{\delta}}{m}},$$

where $u_0 = 1 + \frac{1}{e}$.

Proof

- Proof: by the learning bound for convex ensembles holding uniformly for all ρ, with probability at least $1-\delta$, for all f and $\rho > 0$,

$$R(f) \leq \frac{1}{m} \sum_{i=1}^{m} 1_{\frac{y_i \mathbf{w} \cdot \Phi(x_i)}{\rho \|\mathbf{w}\|_1} - 1 \leq 0} + \frac{4}{\rho} \mathfrak{R}_m(H) + \sqrt{\frac{\log \log_2 \frac{2}{\rho}}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{m}}.$$

- Choosing $\rho = \frac{1}{\|\mathbf{w}\|_1}$ and using $1_{u \leq 1} \leq \log_{u_0}(1 + e^{-u})$ yields immediately the learning bound of the theorem.

Logistic Regression

(Berkson, 1944)

- Logistic model:

$$\Pr[y=+1 \mid x] = \frac{e^{\mathbf{w}\cdot\mathbf{\Phi}(x,+1)}}{Z(x)},$$

where $Z(x) = e^{\mathbf{w}\cdot\mathbf{\Phi}(x,+1)} + e^{\mathbf{w}\cdot\mathbf{\Phi}(x,-1)}$

- Properties:
  - linear decision rule, sign of log-odds ratio:

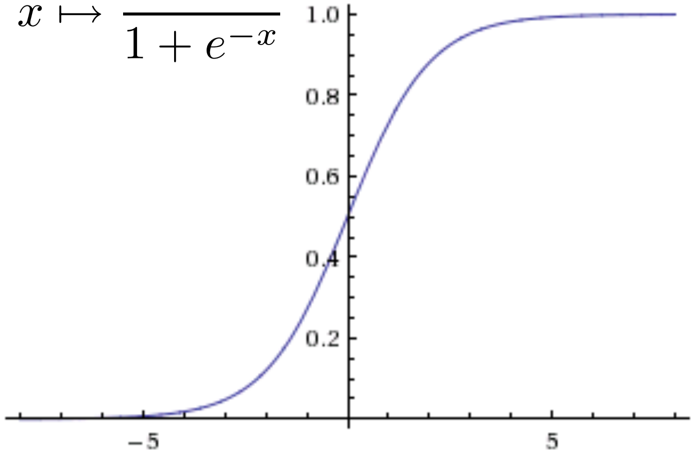
$$\log \frac{\Pr[y=+1 \mid x]}{\Pr[y=-1 \mid x]} = \mathbf{w} \cdot \big(\mathbf{\Phi}(x,+1) - \mathbf{\Phi}(x,-1)\big) = \mathbf{w} \cdot \mathbf{\Psi}(x).$$

  - logistic form:

$$\Pr[y=+1 \mid x] = \frac{1}{1 + e^{-\mathbf{w}\cdot[\mathbf{\Phi}(x,+1)-\mathbf{\Phi}(x,-1)]}} = \frac{1}{1 + e^{-\mathbf{w}\cdot\mathbf{\Psi}(x)}}.$$

Logistic/Sigmoid Function

$$f\colon x \mapsto \frac{1}{1+e^{-x}}$$



$$\Pr[y = +1 \mid x] = f\big(\mathbf{w} \cdot \mathbf{\Psi}(x)\big).$$

Applications

- Natural language processing (Berger et al., 1996; Rosenfeld, 1996; Pietra et al., 1997; Malouf, 2002; Manning and Klein, 2003; Mann et al., 2009; Ratnaparkhi, 2010).
- Species habitat modeling (Phillips et al., 2004, 2006; Dudík et al., 2007; Elith et al, 2011).
- Computer vision (Jeon and Manmatha, 2004).

Extensions

- Extensive theoretical study of alternative regularizations: (Dudík et al., 2007) (see also (Altun and Smola, 2006) though some proofs unclear).
- Maxent models with other Bregman divergences (see for example (Altun and Smola, 2006)).
- Structural Maxent models (Cortes et al., 2015):
    - extension to the case of multiple feature families.
    - empirically outperform Maxent and L1-Maxent.
    - conditional structural Maxent: coincide with deep boosting using the logistic loss.

Conclusion

- Logistic regression/maxent models:
  - theoretical foundation.
  - natural solution when probabilites are required.
  - widely used for density estimation/classification.
  - often very effective in practice.
  - distributed optimization solutions.
  - no natural non-linear L1-version (use of kernels).
  - connections with boosting.
  - connections with neural networks.

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