CS 6347

Lecture 12

Maximum Likelihood Learning

Maximum Likelihood Estimation

- Given samples $x^1, \ldots, x^M$ from some unknown distribution with parameters θ…
  - The log-likelihood of the evidence is defined to be

$$\log l(\theta) = \sum_m \log p(x|\theta)$$

  - Goal: maximize the log-likelihood

MLE for Bayesian Networks

- Given samples $x^1, \ldots, x^M$ from some unknown Bayesian network that factors over the directed acyclic graph G
  - The parameters of a Bayesian model are simply the conditional probabilities that define the factorization
  - For each $i \in G$ we need to learn $p(x_i | x_{parents(i)})$, create a variable $\theta_{x_i | x_{parents(i)}}$

$$\log l(\theta) = \sum_m \sum_{i \in V} \log \theta_{x_i^m | x_{parents(i)}^m}$$

MLE for Bayesian Networks

$$\log l(\theta) = \sum_{m} \sum_{i \in V} \log \theta_{x_i^m | x_{parents(i)}^m}$$

$$= \sum_{i \in V} \sum_{m} \log \theta_{x_i^m | x_{parents(i)}^m}$$

$$= \sum_{i \in V} \sum_{x_{parents(i)}} \sum_{x_i} \mathrm{N}_{x_\mathrm{i}, x_{\mathrm{parents(i)}}} \log \theta_{x_i | x_{parents(i)}}$$

MLE for Bayesian Networks

$$\log l(\theta) = \sum_{m} \sum_{i \in V} \log \theta_{x_i^m | x_{parents(i)}^m}$$

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$N_{x_i, x_{parents(i)}}$ is the number of times $(x_i, x_{parents(i)})$ was observed in the samples

MLE for Bayesian Networks

$$\log l(\theta) = \sum_m \sum_{i \in V} \log \theta_{x_i^m | x_{parents(i)}^m}$$

$$= \sum_{i \in V} \sum_m \log \theta_{x_i^m | x_{parents(i)}^m}$$

$$= \sum_{i \in V} \sum_{x_{parents(i)}} \sum_{x_i} \mathrm{N}_{x_{\mathrm{i}}, x_{\mathrm{parents(i)}}} \log \theta_{x_i | x_{parents(i)}}$$

Fix $x_{parents(i)}$ solve for $\theta_{x_i | x_{parents(i)}}$ for all x_i

(on the board)

MLE for Bayesian Networks

$$\theta_{x_i|x_{parents(i)}} = \frac{\mathrm{N}_{x_i,x_{\text{parents}(i)}}}{\sum_{x_i'} \mathrm{N}_{x_i',x_{\text{parents}(i)}}} = \frac{\mathrm{N}_{x_i,x_{\text{parents}(i)}}}{\mathrm{N}_{x_{\text{parents}(i)}}}$$

- This is just the empirical conditional probability distribution
  - Worked out nicely because of the factorization of the joint distribution
- Similar to the coin flips result from last time

MLE for MRFs

- Let's compute the MLE for MRFs that factor over the graph G as $p(x|\theta) = \frac{1}{Z(\theta)} \prod_C \psi_C(x_C|\theta)$
- The parameters θ control the allowable potential functions
- Again, suppose we have samples $x^1, \ldots, x^M$ from some unknown MRF of this form

$$\log l(\theta) = \left[\sum_m \sum_C \log \psi_C(x_C^m|\theta)\right] - M \log Z(\theta)$$

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$$\log l(\theta) = \left[\sum_m \sum_C \log \psi_C(x_C^m|\theta)\right] - M \log Z(\theta)$$

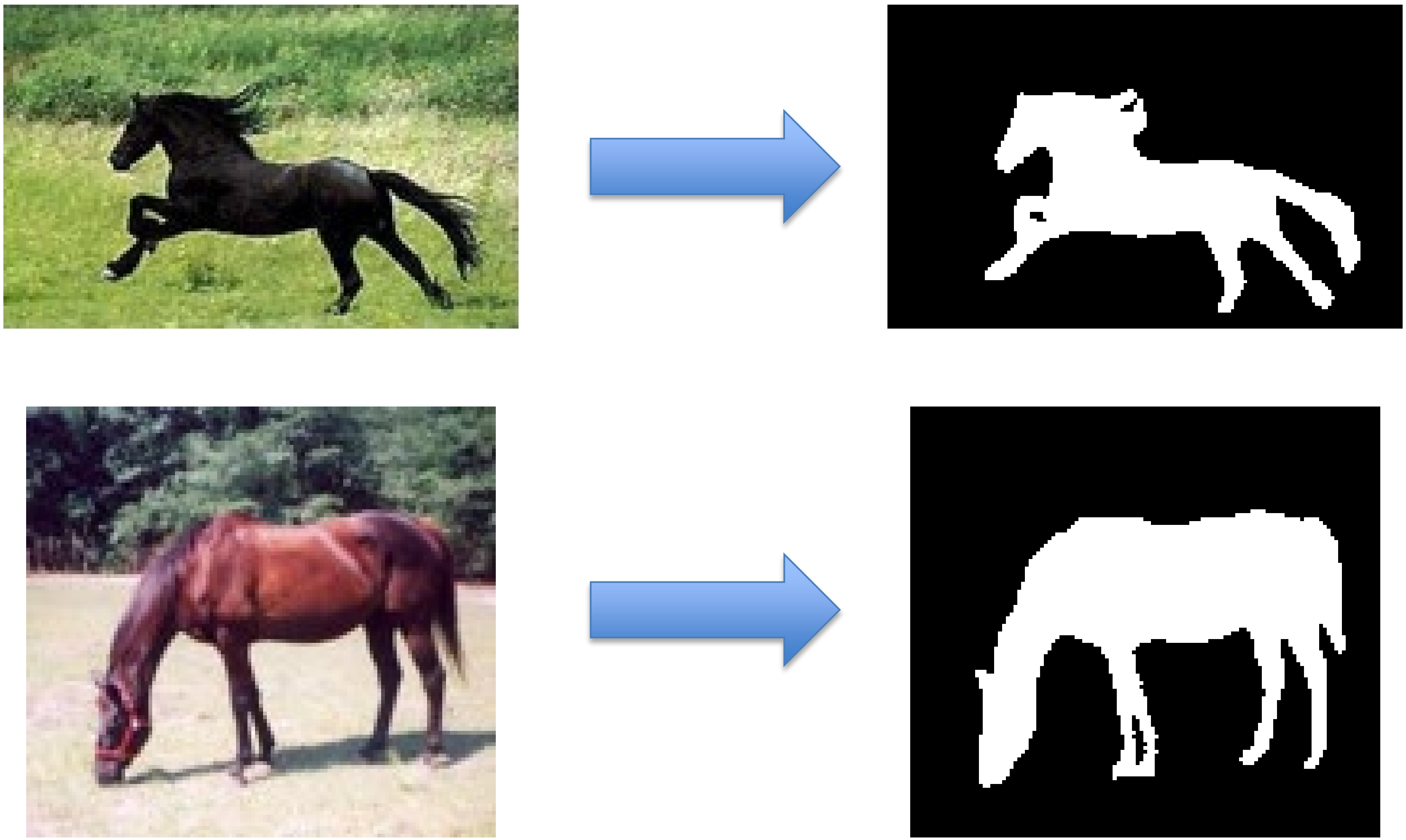
$Z(\theta)$ couples all of the potential functions together!

Even computing $Z(\theta)$ by itself was a challenging task…

Conditional Random Fields

- Learning MRFs is quite restrictive
  - Most "real" problems are really conditional models
- Example: image segmentation
  - Represent a segmentation problem as a MRF over a two dimensional grid
  - Each x_i is an binary variable indicating whether or not the pixel is in the foreground or the background
  - How do we incorporate pixel information?
    - The potentials over the edge (i, j) of the MRF should depend on x_i, x_j as well as the pixel information at nodes i and j

Image Segmentation



Feature Vectors

- The pixel information is called a feature of the model
  - Features will consist of more than just a scalar value (i.e., pixels, at the very least, are vectors of RGBA values)
- Vector of features y (e.g., one vector of features y_i for each $i \in V$)
  - We think of the joint probability distribution as a conditional distribution $p(x|y,\theta)$
- This makes MLE even harder
  - Samples are pairs $(x^1, y^1), \ldots, (x^M, y^M)$
  - The feature vectors can be different for each sample: need to compute $Z(\theta, y^m)$ in the log-likelihood!

Log-Linear Models

- MLE seems daunting for MRFs and CRFs
    - Need a nice way to parameterize the model and to deal with features
- We often assume that the models are log-linear in the parameters
    - Many of the models that we have seen so far can easily be expressed as log-linear models of the parameters
    - Feature vectors should also be incorporated in a log-linear way

Log-Linear Models

- The potential on the clique C should be a log-linear function of the parameters

$$\psi_C(x_C|y,\theta) = \exp(\langle\theta, f_C(x_C,y)\rangle)$$

where

$$\langle\theta, f_C(x_C,y)\rangle = \sum_k \theta_k \cdot f_C(x_C,y)_k$$

- Here, f is a feature map that takes the input variables and returns a vector the same size as θ

Log-Linear MRFs

- Over complete representation: one parameter for each clique C and choice of x_C

$$p(x|\theta) = \frac{1}{Z}\prod_{C} \exp(\theta_C(x_C))$$

  - $f_C(x_C)$ is a 0-1 vector that is indexed by C and x_C whose only non-zero component corresponds to $\theta_C(x_C)$

- One parameter per clique

$$p(x|\theta) = \frac{1}{Z}\prod_{C} \exp(\theta_C f_C(x_C))$$

  - $f_C(x_C)$ is a vector that is indexed ONLY by C whose only non-zero component corresponds to θ_C

MLE for Log-Linear Models

$$p(x|y,\theta) = \frac{1}{Z(\theta, y)} \prod_C \exp(\langle \theta, f_C(x_C, y) \rangle)$$

$$\log l(\theta) = \sum_m \left[\left[\sum_C \langle \theta, f_C(x_C^m, y^m) \rangle \right] - \log Z(\theta, y^m) \right]$$

$$= \left\langle \theta, \sum_m \sum_C f_C(x_C^m, y^m) \right\rangle - \sum_m \log Z(\theta, y^m)$$

MLE for Log-Linear Models

$$p(x|y,\theta) = \frac{1}{Z(\theta,y)} \prod_C \exp(\langle \theta, f_C(x_C, y)\rangle)$$

$$\log l(\theta) = \sum_m \left[\left[\sum_C \langle \theta, f_C(x_C^m, y^m) \rangle \right] - \log Z(\theta, y^m) \right]$$

$$= \underbrace{\left\langle \theta, \sum_m \sum_C f_C(x_C^m, y^m) \right\rangle}_{\text{Linear in } \theta} - \underbrace{\sum_m \log Z(\theta, y^m)}_{\text{Depends non-linearly on } \theta}$$

Concavity of MLE

We will show that $\log Z(\theta, y)$ is a convex function of θ…

Fix a distribution $q(\mathrm{x}|\mathrm{y})$

$$
\begin{aligned}
D(q||p) &= \sum_x q(x|y) \log \frac{q(x|y)}{p(x|y,\theta)} \\
&= \sum_x q(x|y) \log q(x|y) \ - \sum_x q(x|y) \log p(x|y,\theta) \\
&= -H(q) \ - \sum_x q(x|y) \log p(x|y,\theta) \\
&= -H(q) + \log Z(\theta, y) - \sum_x \sum_C q(x|y) \langle \theta, f_C(x_C, y) \rangle \\
&= -H(q) + \log Z(\theta, y) - \sum_C \sum_{x_C} q_C(x_C|y) \langle \theta, f_C(x_C, y) \rangle
\end{aligned}
$$

Concavity of MLE

$$\log Z(\theta, y) = \max_q \left[H(q) + \sum_C \sum_{x_C} \underbrace{q_C(x_C|y)\langle\theta, f_C(x_C, y)\rangle}_{\text{Linear in } \theta} \right]$$

- If a function $g(x, y)$ is convex in x for each y, then $\max_y g(x, y)$ is convex in x
  - As a result, $\log Z(\theta, y)$ is a convex function of θ for a fixed value of y

MLE for Log-Linear Models

$$p(x|y,\theta) = \frac{1}{Z(\theta,y)} \prod_C \exp(\langle \theta, f_C(x_C, y)\rangle)$$

$$\log l(\theta) = \sum_m \left[\left[\sum_C \langle \theta, f_C(x_C^m, y^m)\rangle \right] - \log Z(\theta, y^m) \right]$$

$$= \underbrace{\left\langle \theta, \sum_m \sum_C f_C(x_C^m, y^m) \right\rangle}_{\text{Linear in } \theta} - \underbrace{\sum_m \log Z(\theta, y^m)}_{\text{Convex in } \theta}$$

MLE for Log-Linear Models

$$p(x|y,\theta) = \frac{1}{Z(\theta,y)} \prod_C \exp(\langle \theta, f_C(x_C, y) \rangle)$$

$$\log l(\theta) = \sum_m \left[\left[\sum_C \langle \theta, f_C(x_C^m, y^m) \rangle \right] - \log Z(\theta, y^m) \right]$$

$$= \underbrace{\left\langle \theta, \sum_m \sum_C f_C(x_C^m, y^m) \right\rangle - \sum_m \log Z(\theta, y^m)}_{\text{Concave in } \theta}$$

Could optimize it using gradient ascent!
(need to compute $\nabla_\theta \log Z(\theta, y)$)

MLE via Gradient Ascent

- What is the gradient of the log-likelihood with respect to θ?

$$\nabla_\theta \log Z(\theta, y^m) = ?$$

(worked out on board)

MLE via Gradient Ascent

- What is the gradient of the log-likelihood with respect to θ?

$$\nabla_\theta \log Z(\theta, y^m) = \sum_C \sum_m \sum_{x_C} p_C(x_C | y^m, \theta) f_C(x_C, y^m)$$

This is the expected value of the feature maps under the joint distribution

MLE via Gradient Ascent

- What is the gradient of the log-likelihood with respect to θ?

$$\nabla_\theta \log l(\theta) = \sum_C \sum_m \left(f_C(x_C^m, y^m) - \sum_{x_C} p_C(x_C | y^m, \theta) f_C(x_C, y^m) \right)$$

  - To compute/approximate this quantity, we only need to compute/approximate the marginal distributions $p_C(x_C | y, \theta)$
  - This requires performing marginal inference on a different model at each step of gradient ascent!

Moment Matching

- Let $f(x^m, y^m) = \sum_C f_C(x_C^m, y^m)$
- Setting the gradient with respect to θ equal to zero and solving gives

$$\sum_m f(x^m, y^m) = \sum_m \sum_x p(x|y^m, \theta) f(x, y^m)$$

- This condition is called moment matching and when the model is an MRF instead of a CRF this reduces to

$$\frac{1}{M} \sum_m f(x^m) = \sum_x p(x|\theta) f(x)$$

Moment Matching

- As an example, consider a log-linear MRF

$$p(x) = \frac{1}{Z} \prod_C \exp(\theta_C(x_C))$$

- That is, $f_C(x_C)$ is a vector that is indexed by C and x_C whose only non-zero component corresponds to $\theta_C(x_C)$

- The moment matching condition becomes

$$\frac{1}{M} \sum_m 1_{x_C = x_C^m} = p_C(x_C|\theta), \qquad \text{for all } C, x_C$$

Regularization in MLE

- Recall that we can also incorporate prior information about the parameters into the MLE problem
  - This involved solving an augmented MLE (called MAP estimation)

$$\prod_m p(x^m|\theta)p(\theta)$$

  - What types of priors should we choose for the parameters?

Dirichlet Distribution

- Dirichlet distribution over $x_1, \ldots, x_K$ such that $x_1, \ldots, x_K \geq 0$ and $\sum_i x_i = 1$

$$f(x_1, \ldots, x_K; \alpha_1, \ldots, \alpha_K) \propto \prod_i x_i^{\alpha_i - 1}$$

  - The Dirichlet distribution is a distribution over probability distributions over K elements (generalizes the Beta distribution)

Regularization in MLE

- Recall that we can also incorporate prior information about the parameters into the MLE problem
  - This involved solving an augmented MLE

$$\left[\prod_m p(x^m|\theta)\right] p(\theta)$$

  - What types of priors should we choose for the parameters?
    - Gaussian prior: $p(\theta) \propto \exp(-\frac{1}{2}(\theta - \mu)^T \Sigma^{-1} (\theta - \mu)^T)$
    - Uniform over $[0,1]$

Regularization in MLE

- Recall that we can also incorporate prior information about the parameters into the MLE problem
  - This involved solving an augmented MLE

$$\left[\prod_m p(x^m|\theta)\right] \exp(-\frac{1}{2}\theta^T D\theta)$$

Zero-mean Gaussian prior with a diagonal covariance matrix all of whose entries are equal to λ

  - What types of priors should we choose for the parameters?
    - Gaussian prior: $p(\theta) \propto \exp(-\frac{1}{2}(\theta-\mu)^T\Sigma^{-1}(\theta-\mu)^T)$
    - Uniform over $[0,1]$

Regularization in MLE

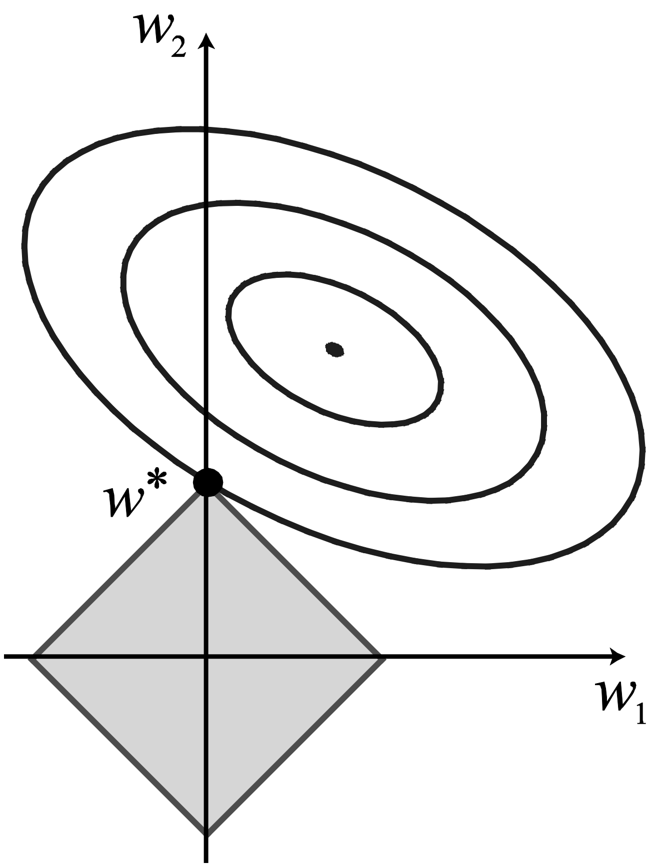
- Using the previous Gaussian prior yields the following log-optimization problem

$$\log\left(\left[\prod_m p(x^m|\theta)\right]\exp(-\frac{1}{2}\theta^T D\theta)\right) = \left[\sum_m \log p(x^m|\theta)\right] - \frac{\lambda}{2}\sum_k \theta_k^2$$

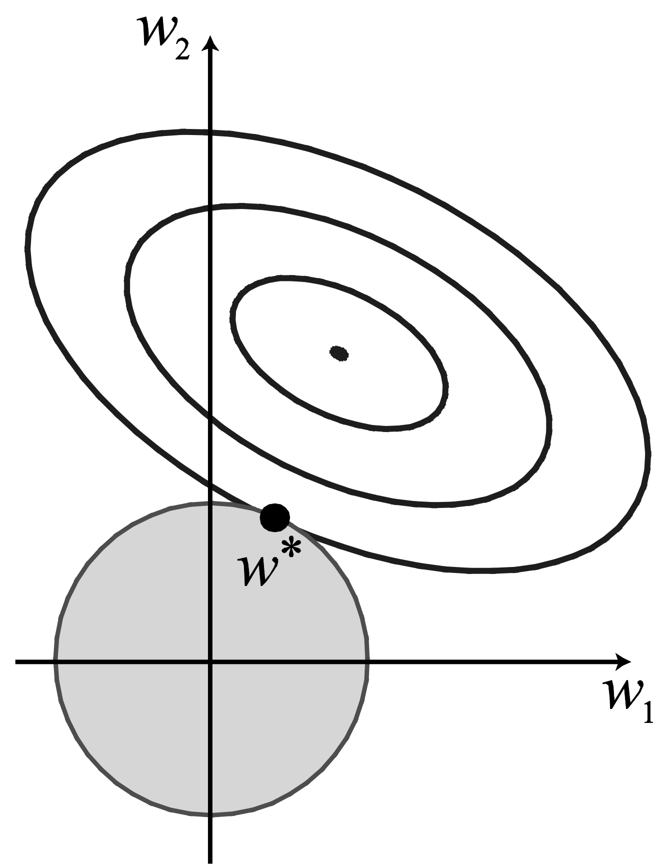
$$= \left[\sum_m \log p(x^m|\theta)\right] - \frac{\lambda}{2}||\theta||_2^2$$

Known as ℓ_2 regularization

Regularization



ℓ_1



ℓ_2

Duality and MLE

$$\log Z(\theta, y) = \max_{q} \left[H(q) + \sum_{C} \sum_{x_C} q_C(x_C|y) \langle \theta, f_C(x_C, y) \rangle \right]$$

$$\log l(\theta) = \left\langle \theta, \sum_{m} \sum_{C} f_C(x_C^m, y^m) \right\rangle - \sum_{m} \log Z(\theta, y^m)$$

Plugging the first into the second gives:

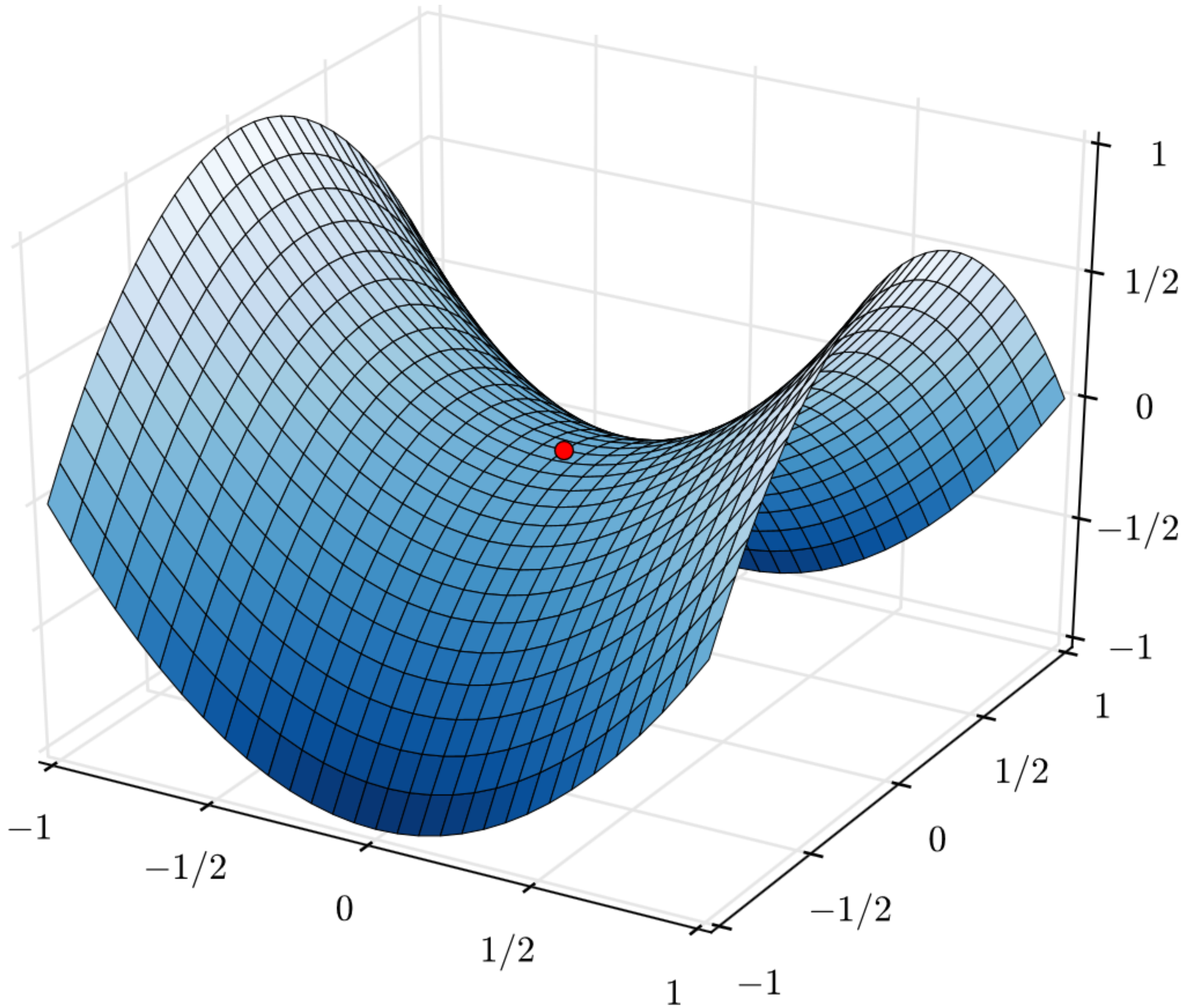
$$\log l(\theta) = \left\langle \theta, \sum_{m} \sum_{C} f_C(x_C^m, y^m) \right\rangle - \sum_{m} \max_{q^m} \left[H(q^m) + \sum_{C} \sum_{x_C} q_C^m(x_C|y^m) \langle \theta, f_C(x_C, y^m) \rangle \right]$$

Duality and MLE

$$\max_{\theta} \log l(\theta) = \max_{\theta} \min_{q^1,\dots,q^M} \left[\left\langle \theta, \sum_C \sum_m \left(f_C(x_C^m, y^m) - \sum_{x_C} q_C^m(x_C|y^m) f_C(x_C, y^m) \right) \right\rangle - \sum_m H(q^m) \right]$$

- This is called a minimax or saddle-point problem
- When can we switch the order of the max and min?
  - The function is linear in theta, so there is an advantage to swapping the order

Saddle Point



Source: Wikipedia

Sion's Minimax Theorem

Let X be a compact convex subset of R^n and Y be a convex subset of R^m

Let f be a real-valued function on $X \times Y$ such that

- $f(x,\cdot)$ a continuous concave function over Y for each $x \in X$
- $f(\cdot,y)$ a continuous convex function over X for each $y \in Y$

then

$$\sup_y \min_x f(x,y) = \min_x \sup_y f(x,y)$$

Duality and MLE

$$\max_{\theta} \min_{q^1,\ldots,q^M} \left[\left\langle \theta, \sum_{C} \sum_{m} \left(f_C(x_C^m, y^m) - \sum_{x_C} q_C^m(x_C|y^m) f_C(x_C, y^m) \right) \right\rangle - \sum_{m} H(q^m) \right]$$

is equal to

$$\min_{q^1,\ldots,q^M} \max_{\theta} \left[\left\langle \theta, \sum_{C} \sum_{m} \left(f_C(x_C^m, y^m) - \sum_{x_C} q_C^m(x_C|y^m) f_C(x_C, y^m) \right) \right\rangle - \sum_{m} H(q^m) \right]$$

Solve for θ?

Maximum Entropy

$$\max_{q^1,\ldots,q^M} \sum_m H(q^m)$$

such that the moment matching condition is satisfied

$$\sum_m f(x^m, y^m) = \sum_m \sum_x q^m(x|y^m) f(x, y^m)$$

and $q^1, \ldots, q^m$ are discrete probability distributions

- Instead of maximizing the log-likelihood, we could maximize the entropy over all approximating distributions that satisfy the moment matching condition

MLE in Practice

- We can compute the partition function in linear time over trees using belief propagation
    - We can use this to learn the parameters of tree-structured models
- What if the graph isn't a tree?
    - Use variable elimination to compute the partition function (exact but slow)
    - Use importance sampling to approximate the partition function (can also be quite slow; maybe only use a few samples?)
    - Use loopy belief propagation to approximate the partition function (can be bad if loopy BP doesn't converge quickly)

MLE in Practice

- Practical wisdom:
  - If you are trying to perform some prediction task (i.e., MAP inference to do prediction), then it is better to learn the "wrong model"
    - Learning and prediction should use the same approximations
- What people actually do:
  - Use a few iterations of loopy BP or sampling to approximate the marginals
  - Approximate marginals give approximate gradients (recall that the gradient only depended on the marginals)
  - Perform approximate gradient descent and hope it works

MLE in Practice

- Other options
  - Replace the true entropy with the Bethe entropy and solve the approximate dual problem
  - Use fancier optimization techniques to solve the problem faster
    - e.g., the method of conditional gradients