# On the likelihood of randomly perturbed max-solutions

Tamir Hazan Technion

• 20 years ago: does an image contain a person?



• 10 years ago: which object is in the image?



• Today's challenge: exponentially many options





- For each pixel: decide if it is foreground or background.
- The space of possible structures is exponential





• Complex structures dominate machine learning applications:

• Complex structures dominate machine learning applications:

- Computer vision



• Complex structures dominate machine learning applications:

- Computer vision



- Natural language processing



• Complex structures dominate machine learning applications:

- Computer vision



- Natural language processing



- and more..

# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.

# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models

# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds

• machine learning applications are characterized by:

- complex structures  $y = (y_1, ..., y_n)$ 

• machine learning applications are characterized by:

- complex structures  $y = (y_1, ..., y_n)$ 

#### $y \in \{0,1\}^n$



• machine learning applications are characterized by:

- complex structures  $y = (y_1, ..., y_n)$ 

- machine learning applications are characterized by:
  - complex structures  $y = (y_1, ..., y_n)$
  - potential function that scores these structures

$$\theta(y_1, \dots, y_n) = \sum_{i \in V} \theta_i(y_i) + \sum_{i,j \in E} \theta_{i,j}(y_i, y_j)$$

- machine learning applications are characterized by:
  - complex structures  $y = (y_1, ..., y_n)$
  - potential function that scores these structures

$$\theta(y_1, \dots, y_n) = \sum_{i \in V} \theta_i(y_i) + \sum_{i,j \in E} \theta_{i,j}(y_i, y_j)$$

#### high score





low score

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

• MCMC samplers:

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang
- Many efficient sampling algorithms for special cases:

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang
- Many efficient sampling algorithms for special cases:
  - Ising models (Jerrum 93)

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang
- Many efficient sampling algorithms for special cases:
  - Ising models (Jerrum 93)
  - Counting bi-partite matchings in planar graphs (Kasteleyn 61)

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang
- Many efficient sampling algorithms for special cases:
  - Ising models (Jerrum 93)
  - Counting bi-partite matchings in planar graphs (Kasteleyn 61)
  - Approximating the permanent (Jerrum 04)

$$p(y_1, \dots, y_n) = \frac{1}{Z} \exp\left(\sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$$

- MCMC samplers:
  - Gibbs sampling, Metropolis-Hastings, Swendsen-Wang
- Many efficient sampling algorithms for special cases:
  - Ising models (Jerrum 93)
  - Counting bi-partite matchings in planar graphs (Kasteleyn 61)
  - Approximating the permanent (Jerrum 04)
  - Many others...

 Gibbs distribution has a significant impact on statistics and computer science

- Gibbs distribution has a significant impact on statistics and computer science
  - Efficient sampling in Ising models (Jerrum 93)

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

- Gibbs distribution has a significant impact on statistics and computer science
  - Efficient sampling in Ising models (Jerrum 93)
  - Attractive pairwise potentials

$$\theta_{i,j}(y_i, y_j) = \begin{cases} w_{i,j} & \text{if } y_i = y_j \\ -w_{i,j} & \text{otherwise} \end{cases}$$

 $w_{i,j} \ge 0$ 

- No data terms

 $\theta_i(y_i) = 0$ 

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

- Gibbs distribution has a significant impact on statistics and computer science
  - Efficient sampling in Ising models (Jerrum 93)
  - Attractive pairwise potentials

$$\theta_{i,j}(y_i, y_j) = \begin{cases} w_{i,j} & \text{if } y_i = y_j \\ -w_{i,j} & \text{otherwise} \end{cases}$$

 $w_{i,j} \ge 0$ 

- No data terms

 $\theta_i(y_i) = 0$ 

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

- Gibbs distribution has a significant impact on statistics and computer science
  - Efficient sampling in Ising models (Jerrum 93)
  - Attractive pairwise potentials

$$\theta_{i,j}(y_i, y_j) = \begin{cases} w_{i,j} & \text{if } y_i = y_j \\ -w_{i,j} & \text{otherwise} \end{cases}$$

 $w_{i,j} \ge 0$ 

- No data terms

 $\theta_i(y_i) = 0$ 

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

 Nicely behaved distribution that is centered around the (1,...,1) or (0,...,0)

Sampling likely structures may easily handle ambiguities



Sampling likely structures may easily handle ambiguities



• Sampling likely structures may easily handle inaccurate modeling

Sampling likely structures may easily handle inaccurate modeling



Sampling likely structures may easily handle inaccurate modeling






Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, Jerrum 93)

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

 Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, Jerrum 93)



•  $x_i$  RGB color of pixel i  $\theta_i(y_i) = \log q(y_i|x_i)$ 

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

 Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, Jerrum 93)



•  $x_i$  RGB color of pixel i  $\theta_i(y_i) = \log q(y_i|x_i)$ 

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$



 Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, Jerrum 93)

$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$

 $\mathbf{N}$ 

 $\theta_i(y_i) = \log q(y_i|x_i)$ 

 Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, lerrum 93)



 $p(y) \propto \exp\left(\sum_{i} \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)\right)$ 

 $\theta_i(y_i) = \log q(y_i|x_i)$ 

 Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, lerrum 93)



 $\theta_i(y_i) = \log q(y_i|x_i)$ 

 Recall: sampling from the Gibbs distribution is easy in Ising models (Jerrum 93)



- Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, lerrum 93)
  - 0.1 0.4 0.09 0.35 0.08 0.3 0.07 0.25 0.06 0.05 0.2 0.04 0.15 0.03 0.1 0.02 0.05 0.01 003 100 200 300 400 500 600  $\theta_i(y_i) = 0$  $\theta_i(y_i) = \log q(y_i|x_i)$
- Recall: sampling from the Gibbs distribution is easy in Ising models (Jerrum 93)

- Sampling from the Gibbs distribution is provably hard in Al applications (Goldberg 05, lerrum 93)
- Recall: sampling from the Gibbs distribution is easy in Ising models (Jerrum 93)



 Instead of sampling, it may be significantly faster to find the most likely structure

 Instead of sampling, it may be significantly faster to find the most likely structure



- Instead of sampling, it may be significantly faster to find the most likely structure
  - Graph-cuts



- Instead of sampling, it may be significantly faster to find the most likely structure
  - Graph-cuts

$$\theta_{i,j}(y_i, y_j) = \begin{cases} w_{i,j} & \text{if } y_i = y_j \\ -w_{i,j} & \text{otherwise} \end{cases}$$
$$w_{i,j} \ge 0$$

 $\theta_i(y_i) = \log q(y_i|x_i)$ 



- Instead of sampling, it may be significantly faster to find the most likely structure
  - Graph-cuts

$$\theta_{i,j}(y_i, y_j) = \begin{cases} w_{i,j} & \text{if } y_i = y_j \\ -w_{i,j} & \text{otherwise} \end{cases}$$
$$w_{i,j} \ge 0$$

 $\theta_i(y_i) = \log q(y_i|x_i)$ 





$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

• Maximum a-posteriori (MAP) inference.

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),
  - Graph-cuts for image segmentation

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),
  - Graph-cuts for image segmentation
  - branch and cut (Gurobi), local consistency (Larrosa 03, de Givry 05), mini-buckets (Dechter 97)

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),
  - Graph-cuts for image segmentation
  - branch and cut (Gurobi), local consistency (Larrosa 03, de Givry 05), mini-buckets (Dechter 97)
  - Linear programming relaxations (Schlesinger 76, Wainwright 05, Kolmogorov 06, Komodakis 07, Werner 07, Sontag 08, Hazan 10, Kappes 13, Savchynskyy13, Tarlow 13)

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),
  - Graph-cuts for image segmentation
  - branch and cut (Gurobi), local consistency (Larrosa 03, de Givry 05), mini-buckets (Dechter 97)
  - Linear programming relaxations (Schlesinger 76, Wainwright 05, Kolmogorov 06, Komodakis 07, Werner 07, Sontag 08, Hazan 10, Kappes 13, Savchynskyy13, Tarlow 13)
  - CKY for parsing

$$y^* = \arg \max_{y_1, \dots, y_n} \sum_i \theta_i(y_i) + \sum_{i,j} \theta_{i,j}(y_i, y_j)$$

- Maximum a-posteriori (MAP) inference.
- Many efficient optimization algorithms for special cases:
  - Beliefs propagation: trees (Pearl 88), perfect graphs (Jebara 10),
  - Graph-cuts for image segmentation
  - branch and cut (Gurobi), local consistency (Larrosa 03, de Givry 05), mini-buckets (Dechter 97)
  - Linear programming relaxations (Schlesinger 76, Wainwright 05, Kolmogorov 06, Komodakis 07, Werner 07, Sontag 08, Hazan 10, Kappes 13, Savchynskyy13, Tarlow 13)
  - CKY for parsing
  - Many others...

#### The challenge

Sampling from the likely high dimensional structures (with millions of variables, e.g., image segmentation with 12 million pixels) as efficient as optimizing























Randomly perturbing the system reveals its complexity



- Randomly perturbing the system reveals its complexity
  - little effect when the maximizing structure is "evident"



- Randomly perturbing the system reveals its complexity
  - little effect when the maximizing structure is "evident"

#### Random perturbations



- Randomly perturbing the system reveals its complexity
  - little effect when the maximizing structure is "evident"
  - substantial effect when there are alternative high scoring structures
# scores

Randomly perturbing the system reveals its complexity

structures

- little effect when the maximizing structure is "evident"

structures

 $y^*$ 

 substantial effect when there are alternative high scoring structures

# scores $f_{y^*}$ structures structures $y^*$

- Randomly perturbing the system reveals its complexity
  - little effect when the maximizing structure is "evident"
  - substantial effect when there are alternative high scoring structures



- Randomly perturbing the system reveals its complexity
  - little effect when the maximizing structure is "evident"
  - substantial effect when there are alternative high scoring structures
- Related work:
  - McFadden 74 (Discrete choice theory)
  - Talagrand 94 (Canonical processes)







### • Notation:





### • Notation:





• Notation:



• For every structure y, the perturbation value  $\gamma(y)$  is a random variable (y is an index, traditional notation is  $\gamma_y$ ).



- For every structure y, the perturbation value  $\gamma(y)$  is a random variable (y is an index, traditional notation is  $\gamma_y$ ).
- Perturb-max models: how stable is the maximal structure to random changes in the potential function.



# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds



### Theorem

Let  $\gamma(y)$  be i.i.d. with Gumbel distribution with zero mean

$$F(t) \stackrel{def}{=} P[\gamma(y) \le t] = \exp(-\exp(-t))$$

### Theorem



Let  $\gamma(y)$  be i.i.d. with Gumbel distribution with zero mean

$$F(t) \stackrel{def}{=} P[\gamma(y) \le t] = \exp(-\exp(-t))$$
$$f(t) = F'(t) = \exp(-t)F(t)$$





### Theorem

Let  $\gamma(y)$  be i.i.d. with Gumbel distribution with zero mean

$$F(t) \stackrel{def}{=} P[\gamma(y) \le t] = \exp(-\exp(-t))$$

### Theorem



Let  $\gamma(y)$  be i.i.d. with Gumbel distribution with zero mean

$$F(t) \stackrel{def}{=} P[\gamma(y) \le t] = \exp(-\exp(-t))$$

then the perturb-max model is the Gibbs distribution

$$\frac{1}{Z} \exp(\theta(y)) = P_{\gamma \sim Gumbel} [y = \arg \max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

Let  $\gamma(y)$  be i.i.d Gumbel (  $P[\gamma(y) \leq t] = F(t)$  ). Then

 $\max_{y} \{\theta(y) + \gamma(y)\}$ 

- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

Let  $\gamma(y)$  be i.i.d Gumbel (  $P[\gamma(y) \leq t] = F(t)$  ). Then



- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

Let  $\gamma(y)$  be i.i.d Gumbel (  $P[\gamma(y) \leq t] = F(t)$  ). Then

 $\max_{y} \{\theta(y) + \gamma(y)\}$ 

- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

Let  $\gamma(y)$  be i.i.d Gumbel (  $P[\gamma(y) \leq t] = F(t)$  ). Then

 $\max_{y} \{\theta(y) + \gamma(y)\}$ 

• Proof: 
$$P_{\gamma}[\max_{y} \{\theta(y) + \gamma(y)\} \le t] = \prod_{y} F(t - \theta(y))$$

- Why Gumbel distribution?  $F(t) = \exp(-\exp(-t))$
- Since maximum of Gumbel variables is a Gumbel variable.

Let  $\gamma(y)$  be i.i.d Gumbel (  $P[\gamma(y) \leq t] = F(t)$  ). Then

 $\max_{y} \{\theta(y) + \gamma(y)\}$ 

• Proof: 
$$P_{\gamma}[\max_{y} \{\theta(y) + \gamma(y)\} \le t] = \prod_{y} F(t - \theta(y))$$
$$= \exp(-\sum_{y} \exp(-(t - \theta(y)))) = F(t - \log Z)$$



• Max stability:

$$\log\left(\sum_{y} \exp(\theta(y))\right) = E_{\gamma \sim Gumbel} \left[\max_{y} \{\theta(y) + \gamma(y)\}\right]$$

• Implications (taking gradients):



• Max stability:

$$\log\left(\sum_{y} \exp(\theta(y))\right) = E_{\gamma \sim Gumbel} \left[\max_{y} \{\theta(y) + \gamma(y)\}\right]$$

• Implications (taking gradients):

$$\frac{1}{Z} \exp(\theta(y)) = P_{\gamma \sim Gumbel}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$y = (y_1, \dots, y_n)$$

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$y = (y_1, \dots, y_n)$$



$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$y = (y_1, \dots, y_n)$$

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

$$y = (y_1, \dots, y_n)$$



 Representing the Gibbs distribution using perturb-max models may require exponential number of perturbations

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \gamma(\hat{y})\}]$$

 Use low dimension perturbations (Papandreou & Yuille 11, Tarlow et al. 12, Hazan & Jaakkola 12)

$$P_{\gamma}[y = \arg\max_{\hat{y}} \{\theta(\hat{y}) + \sum_{i=1}^{n} \gamma_i(\hat{y}_i)\}]$$

# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds

The marginal polytope  

$$\theta(y_1, ..., y_n) = \sum_{i \in V} \theta_i(y_i) + \sum_{i,j \in E} \theta_{i,j}(y_i, y_j)$$















$$\mu = \begin{pmatrix} \mu_1(0), \mu_1(1), \mu_2(0), \mu_2(1), \mu_3(0), \mu_3(1), \\ \mu_{1,2}(0,0), \mu_{1,2}(0,1), \mu_{1,2}(1,0), \mu_{1,2}(1,1), \\ \mu_{2,3}(0,0), \mu_{2,3}(0,1), \mu_{2,3}(1,0), \mu_{2,3}(1,1)) \end{pmatrix}$$




$$\mu = \left(\begin{array}{c} \mu_1(0), \mu_1(1), \mu_2(0), \mu_2(1), \mu_3(0), \mu_3(1), \\ \mu_{1,2}(0,0), \mu_{1,2}(0,1), \mu_{1,2}(1,0), \mu_{1,2}(1,1), \\ \mu_{2,3}(0,0), \mu_{2,3}(0,1), \mu_{2,3}(1,0), \mu_{2,3}(1,1)) \end{array}\right)$$

$$\exists p(y_1, y_2, y_3) \text{ s.t. } \mu_1(y_1) = \sum_{y_2, y_3} p(y_1, y_2, y_3), \dots$$
$$\mu_{1,2}(y_1, y_2) = \sum_{y_3} p(y_1, y_2, y_3), \dots$$



$$p(y) \propto \exp\left(\sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j})\right)$$











$$p(y) = P_{\gamma} \left[ y = \arg \max_{y} \left\{ \sum_{i} \theta_{i}(y_{i}) + \sum_{i,j} \theta_{i,j}(y_{i}, y_{j}) + \sum_{i} \gamma_{i}(y_{i}) \right\} \right]$$













# Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds



• Gibbs distribution is defined by its Markov property: a variable is independent of the rest given its neighbors

• Gibbs distribution is defined by its Markov property: a variable is independent of the rest given its neighbors



- Gibbs distribution is defined by its Markov property: a variable is independent of the rest given its neighbors
  - Used in Gibbs sampling, Belief propagation etc.



- Gibbs distribution is defined by its Markov property: a variable is independent of the rest given its neighbors
  - Used in Gibbs sampling, Belief propagation etc.



• What is the modeling power of perturb-max models ?

- Gibbs distribution is defined by its Markov property: a variable is independent of the rest given its neighbors
  - Used in Gibbs sampling, Belief propagation etc.



- What is the modeling power of perturb-max models ?
- Can they model dependencies beyond graph neighborhoods?

# Long range dependencies



• Graphical model whose vertices are the joints.

# Long range dependencies



• Graphical model whose vertices are the joints.

 With Gibbs distribution the arm movements are independent of the legs given the body.

# Long range dependencies



Graphical model whose vertices are the joints.

- With Gibbs distribution the arm movements are independent of the legs given the body.
- Perturb-max can model these long range dependencies (e.g., legs / arms dependencies).

$$p(y_1, y_2, y_3) = \frac{1}{Z} \exp\left(\theta_{1,2}(y_1, y_2) + \theta_{2,3}(y_2, y_3)\right)$$

$$p(y_1, y_2, y_3) = \frac{1}{Z} \exp\left(\theta_{1,2}(y_1, y_2) + \theta_{2,3}(y_2, y_3)\right)$$

• Conditional independence:

 $p(y_1, y_3|y_2) = p(y_1|y_2)p(y_3|y_2)$ 

$$p(y_1, y_2, y_3) = \frac{1}{Z} \exp\left(\theta_{1,2}(y_1, y_2) + \theta_{2,3}(y_2, y_3)\right)$$

• Conditional independence:

 $p(y_1, y_3 | y_2) = p(y_1 | y_2) p(y_3 | y_2)$ 

• Probability of intersection = product of probabilities

$$p(y_1, y_2, y_3) = \frac{1}{Z} \exp\left(\theta_{1,2}(y_1, y_2) + \theta_{2,3}(y_2, y_3)\right)$$

Conditional independence:

 $p(y_1, y_3 | y_2) = p(y_1 | y_2) p(y_3 | y_2)$ 

#### Probability of intersection = product of probabilities



 $P[y_1, y_2, y_3] = P_{\gamma}[y = \arg\max_{\hat{y}} \{\sum_{i,j} \theta_{i,j}(\hat{y}_i, \hat{y}_j) + \gamma_{i,j}(\hat{y}_i, \hat{y}_j)\}]$ 

$$P[y_1, y_2, y_3] = P_{\gamma}[y = \arg\max_{\hat{y}} \{\sum_{i,j} \theta_{i,j}(\hat{y}_i, \hat{y}_j) + \gamma_{i,j}(\hat{y}_i, \hat{y}_j)\}]$$

 max-value flows in perturb-max models incorporate longrange interactions when using independent perturbations

$$P[y_1, y_2, y_3] = P_{\gamma}[y = \arg\max_{\hat{y}} \{\sum_{i,j} \theta_{i,j}(\hat{y}_i, \hat{y}_j) + \gamma_{i,j}(\hat{y}_i, \hat{y}_j)\}]$$

 max-value flows in perturb-max models incorporate longrange interactions when using independent perturbations

$$P[y_1, y_3 | y_2] \neq P[y_1 | y_2] P[y_3 | y_2]$$

$$P[y_1, y_2, y_3] = P_{\gamma}[y = \arg\max_{\hat{y}} \{\sum_{i,j} \theta_{i,j}(\hat{y}_i, \hat{y}_j) + \gamma_{i,j}(\hat{y}_i, \hat{y}_j)\}]$$

 max-value flows in perturb-max models incorporate longrange interactions when using independent perturbations

 $P[y_1, y_3 | y_2] \neq P[y_1 | y_2] P[y_3 | y_2]$ 



• Proof idea: although fixing  $y_2$  decomposes the max, information about the max-value flows.

• Proof idea: although fixing  $y_2$  decomposes the max, information about the max-value flows.

 $\max_{\hat{y}_1, \hat{y}_3} \{ \theta_{1,2}(\hat{y}_1, y_2) + \gamma_{1,2}(\hat{y}_1, y_2) + \theta_{2,3}(y_2, \hat{y}_3) + \gamma_{2,3}(y_2, \hat{y}_3) \} =$ 

• Proof idea: although fixing  $y_2$  decomposes the max, information about the max-value flows.

$$\max_{\hat{y}_1, \hat{y}_3} \{ \theta_{1,2}(\hat{y}_1, y_2) + \gamma_{1,2}(\hat{y}_1, y_2) + \theta_{2,3}(y_2, \hat{y}_3) + \gamma_{2,3}(y_2, \hat{y}_3) \} = \\ \max_{\hat{y}_1} \{ \theta_{1,2}(\hat{y}_1, y_2) + \gamma_{1,2}(\hat{y}_1, y_2) \} + \max_{\hat{y}_3} \{ \theta_{2,3}(y_2, \hat{y}_3) + \gamma_{2,3}(y_2, \hat{y}_3) \}$$

• Proof idea: although fixing  $y_2$  decomposes the max, information about the max-value flows.

$$\begin{split} &\max_{\hat{y}_1, \hat{y}_3} \{\theta_{1,2}(\hat{y}_1, y_2) + \gamma_{1,2}(\hat{y}_1, y_2) + \theta_{2,3}(y_2, \hat{y}_3) + \gamma_{2,3}(y_2, \hat{y}_3)\} = \\ &\max_{\hat{y}_1} \{\theta_{1,2}(\hat{y}_1, y_2) + \gamma_{1,2}(\hat{y}_1, y_2)\} + \max_{\hat{y}_3} \{\theta_{2,3}(y_2, \hat{y}_3) + \gamma_{2,3}(y_2, \hat{y}_3)\} \\ &\bullet \text{High } \gamma_{1,2}(y_1, y_2) \text{ will allow more values of } \gamma_{2,3}(y_2, y_3) \end{split}$$
#### Perturb-max models

• Proof idea: although fixing  $y_2$  decomposes the max, information about the max-value flows.

$$\begin{split} &\max_{\hat{y}_1,\hat{y}_3} \{\theta_{1,2}(\hat{y}_1,y_2) + \gamma_{1,2}(\hat{y}_1,y_2) + \theta_{2,3}(y_2,\hat{y}_3) + \gamma_{2,3}(y_2,\hat{y}_3)\} = \\ &\max_{\hat{y}_1} \{\theta_{1,2}(\hat{y}_1,y_2) + \gamma_{1,2}(\hat{y}_1,y_2)\} + \max_{\hat{y}_3} \{\theta_{2,3}(y_2,\hat{y}_3) + \gamma_{2,3}(y_2,\hat{y}_3)\} \\ &\bullet \text{High } \gamma_{1,2}(y_1,y_2) \text{ will allow more values of } \gamma_{2,3}(y_2,y_3) \end{split}$$



### Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds

 $\bullet$  Given training data  $S\,$  of observed structures

 $\bullet$  Given training data  $S\,$  of observed structures

– e.g., foreground background segmentations  $\ y \in S$ 

オネトスホイ

 $\bullet$  Given training data  $S\,$  of observed structures

– e.g., foreground background segmentations  $\ y \in S$ 

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

 $\bullet$  Given training data  $S\,$  of observed structures

– e.g., foreground background segmentations  $\ y \in S$ 

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$

• Examples

- Learning segmentation potentials

$$y_i \in \{-1, 1\}$$



• Examples

- Learning segmentation potentials  $y_i$ 

$$y_i \in \{-1, 1\}$$



$$\theta_i(y_i;\gamma_i) = \gamma_i y_i$$

$$\theta_{i,j}(y_i, y_j; \gamma_{i,j}) = \begin{cases} \gamma_{i,j} & \text{if } y_i = y_j \\ -\gamma_{i,j} & \text{otherwise} \end{cases}$$

• Examples

- Learning segmentation potentials  $y_i$ 

$$y_i \in \{-1, 1\}$$



$$\theta_i(y_i;\gamma_i) = \gamma_i y_i$$

$$\theta_{i,j}(y_i, y_j; \gamma_{i,j}) = \begin{cases} \gamma_{i,j} & \text{if } y_i = y_j \\ -\gamma_{i,j} & \text{otherwise} \end{cases}$$

General notation:

 $\theta_{\alpha}(y_{\alpha};\gamma_{\alpha}) = \gamma_{\alpha}\phi_{\alpha}(y_{\alpha})$ 

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

• Key fact: the perturb-max models are convolutions

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

log-concave

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$
$$\frac{\text{strongly}}{\text{log-concave}}$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w) \qquad \text{strongly concave} \Rightarrow \text{generalize well}$$

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$
$$strongly \\ \log\text{-concave} \qquad \log\text{-concave}$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w) \qquad \text{strongly concave} \Rightarrow \text{generalize well}$$

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w) \qquad \text{strongly concave} \Rightarrow \text{generalize well}$$

• Key fact: the perturb-max models are convolutions

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) 1 \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

non-smooth

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w) \qquad \text{strongly concave} \Rightarrow \text{generalize well}$$

• Key fact: the perturb-max models are convolutions

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) \mathbb{1} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

smooth

non-smooth

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

 $\max_{w} \sum_{y \in S} \log p(y; w) \qquad \text{strongly concave} \Rightarrow \text{generalize well} \\ \text{smooth (vanishing gradient} \Rightarrow \text{optimum})$ 

• Key fact: the perturb-max models are convolutions

$$p(y;w) = P_{\gamma \sim q_w} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right]$$
$$= \int q_w(\gamma) \mathbb{1} \left[ y = \arg \max_{\hat{y}} \left\{ \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha};\gamma_{\alpha}) \right\} \right] d\gamma$$

smooth

non-smooth

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

Gradients match between prior and posterior predictions

$$\frac{\partial \sum_{y \in S} \log p(y; w)}{\partial w} = \sum_{y \in S} \left( E \left[ \gamma \mid y = \arg \max_{\hat{y}} \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha}; \gamma_{\alpha}) \right] - w \right)$$

 $\bullet$  Learn the parameters w that maximize the perturb-max likelihood

$$\max_{w} \sum_{y \in S} \log p(y; w)$$

Gradients match between prior and posterior predictions

$$\frac{\partial \sum_{y \in S} \log p(y; w)}{\partial w} = \sum_{y \in S} \left( E \left[ \gamma \mid y = \arg \max_{\hat{y}} \sum_{\alpha} \theta_{\alpha}(\hat{y}_{\alpha}; \gamma_{\alpha}) \right] - w \right)$$

 When using log-concave perturbations the deviation of sampled average from the expectation decays exponentially (Orabona, Hazan, Sarwate, Jaakkola 14)

### Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds

• Use perturb-max models to sample possible annotations and estimate user clicks [Maji, Hazan, Jaakkola 14]



 Use perturb-max models to sample possible annotations and estimate user clicks



 Use perturb-max models to sample possible annotations and estimate user clicks



Choose an area with the largest uncertainty reduction

$$U(p_{\theta}) = E_{\gamma} \left[ \sum_{i=1}^{n} \gamma_i(y_i^*) \right] \qquad \qquad y^* = \arg \max_{\hat{y}} \left\{ \theta(\hat{y}) + \sum_{i=1}^{n} \gamma_i(\hat{y}_i) \right\}$$



#### **Online Learning**

• How to choose your route to work?



 Choosing your route daily using perturb-max models is as good (on average) as choosing the best route [Kalai & Vempala 05, Cohen & Hazan 15]

#### Loss minimization

• Can we learn from a finite sample set and generalize?



• Minimizing the average loss using perturb-max models generalize well [Hazan et al. 13]

### Outline

- Random perturbation why and how?
  - Sampling likely structures as fast as finding the most likely one.
- Connections and Alternatives to Gibbs distribution:
  - the marginal polytope
  - the modeling power of perturb-max models
- Learning with perturb-max models
  - log-likelihood learning
  - interactive learning using new entropy bounds
  - online learning
  - loss minimization and PAC-Bayesian bounds

• Perturb-max models:

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?
  - How do the perturbations dimension affect the model properties?

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?
  - How do the perturbations dimension affect the model properties?
  - In what ways higher dimension perturbations reveal complex structures in the model?

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?
  - How do the perturbations dimension affect the model properties?
  - In what ways higher dimension perturbations reveal complex structures in the model?
  - How to apply perturbations in restricted spaces, e.g., super-modular potential functions?
## **Open problems**

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?
  - How do the perturbations dimension affect the model properties?
  - In what ways higher dimension perturbations reveal complex structures in the model?
  - How to apply perturbations in restricted spaces, e.g., super-modular potential functions?
  - How to encourage diverse sampling?

## **Open problems**

- Perturb-max models:
  - When does fixing variables in the max-function amount to statistical conditioning?
  - When do perturb-max models preserve the most likely assignment?
  - How do the perturbations dimension affect the model properties?
  - In what ways higher dimension perturbations reveal complex structures in the model?
  - How to apply perturbations in restricted spaces, e.g., super-modular potential functions?
  - How to encourage diverse sampling?

## Thank you

