

Minimizing Probability Flow

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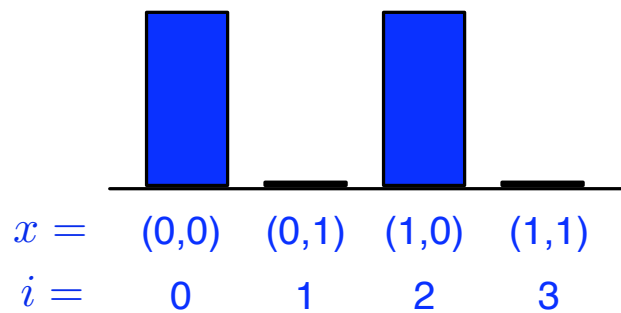
CIFAR Neural Computation and Adaptive Perception Summer School

Aug 12, 2010

University of Toronto

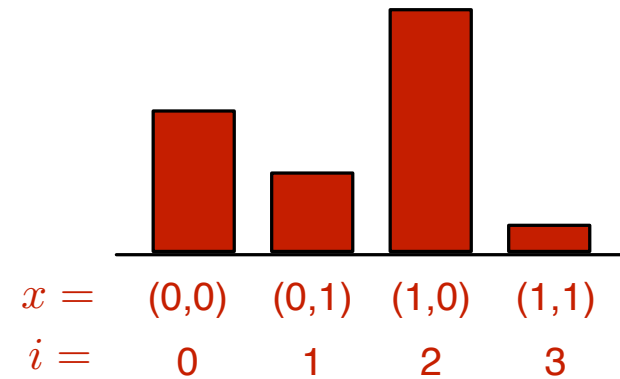
Learning in probabilistic models...

- Want to fit a parametric model to data



data distribution

$$p_i^{(0)} = \text{fraction data in state } i$$



model distribution

$$p_i^{(\infty)}(\theta) = \frac{e^{-E_i(\theta)}}{Z(\theta)}$$

$$Z(\theta) = \sum_i e^{-E_i(\theta)}$$

- Adjust θ so the model distribution looks like the data distribution

Learning in probabilistic models... ...is hard

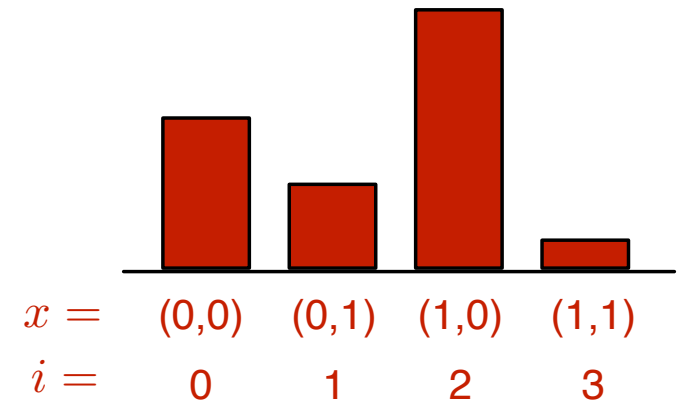
- Maximum likelihood

$$\begin{aligned} K_{ML} &= - \sum_i p_i^{(0)} \log p_i^{(\infty)}(\theta) \\ &= \sum_i p_i^{(0)} E_i(\theta) + \log Z(\theta) \end{aligned}$$

- For a 100 bit binary system

$$Z(\theta) = \sum_{i=1}^{2^{100}} e^{-E_i(\theta)}$$

$$2^{100} = 1267650600228229401496703205376$$



model distribution

$$p_i^{(\infty)}(\theta) = \frac{e^{-E_i(\theta)}}{Z(\theta)}$$

$$Z(\theta) = \sum_i e^{-E_i(\theta)}$$

Existing Techniques

- Numerical integration, Monte Carlo sampling, mean field theory, variational bayes, pseudo likelihood, Ratio Matching, Noise Contrastive Estimation...

- Contrastive Divergence

GE Hinton. Training products of experts by minimizing contrastive divergence. *Neural Computation* (2002)

- Score Matching

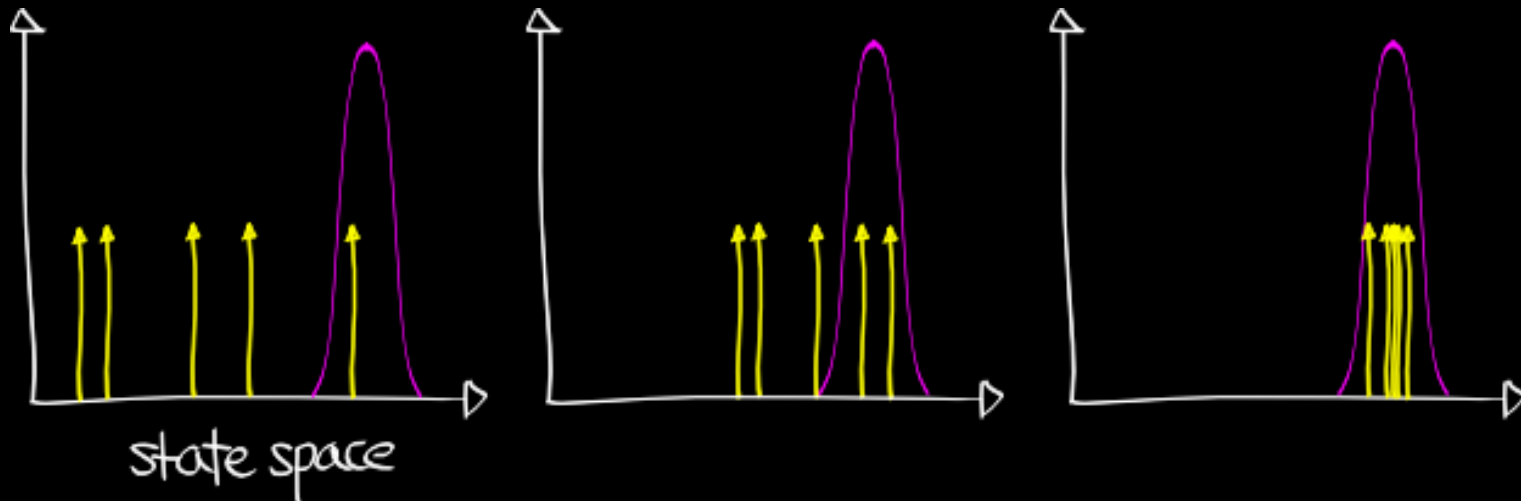
A Hyvärinen. Estimation of non-normalized statistical models using score matching. *Journal of Machine Learning Research*, 6:695–709, 2005.

- Minimum Velocity learning

J R Movellan. A minimum velocity approach to learning. *unpublished draft*, Jan 2008.

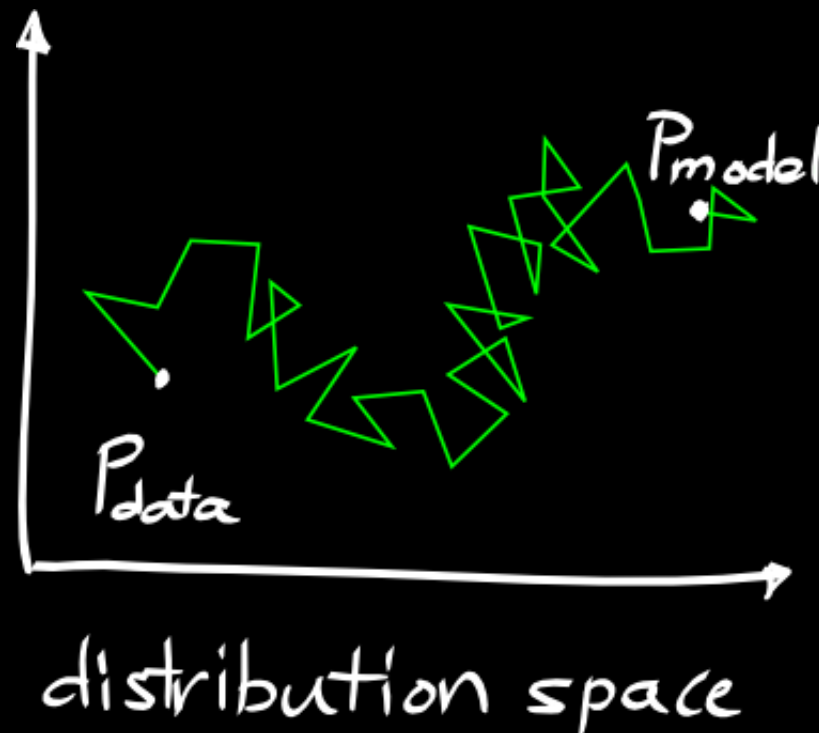
MPF Overview

- Sampling from a distribution:
- Take a set of samples and apply a series of stochastic transformations to it until it looks like it came from the model distribution



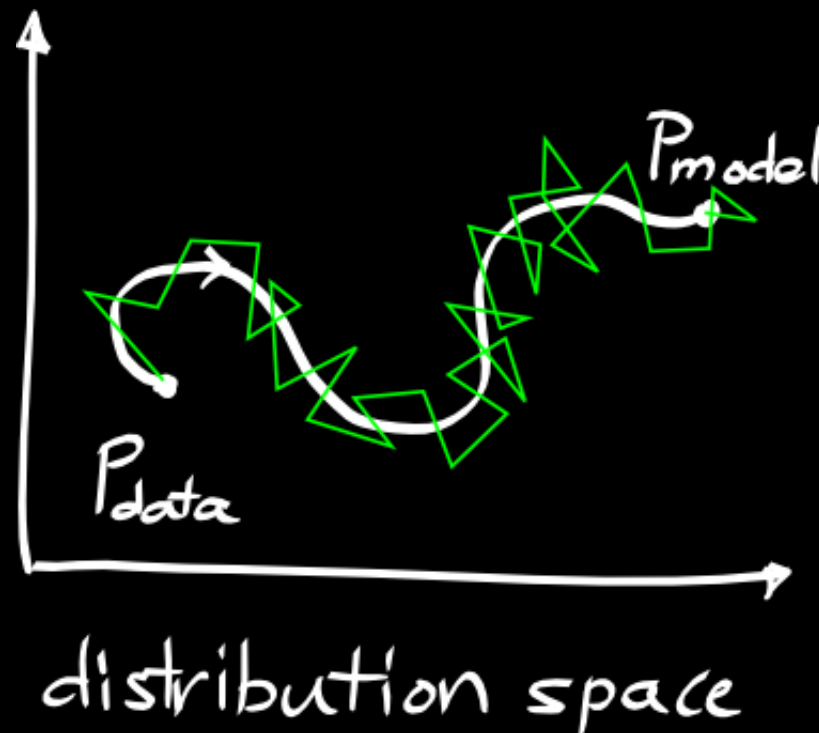
MPF Overview

- Problem with sampling:
 - **SLOW** to converge for large, high-dimensional data sets



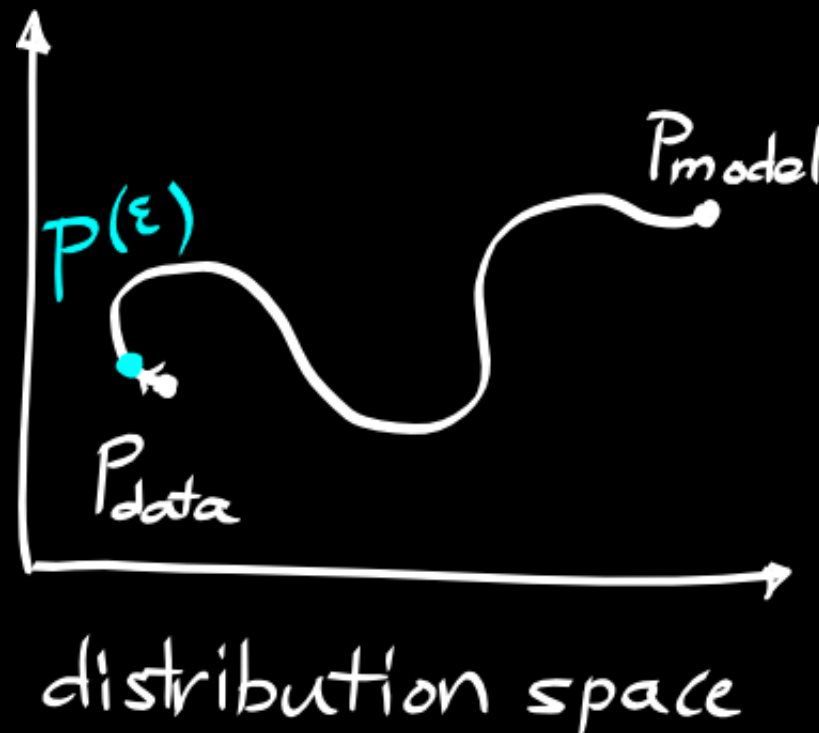
MPF Overview

- Idea: introduce deterministic dynamics interpolating between the data and model distributions...

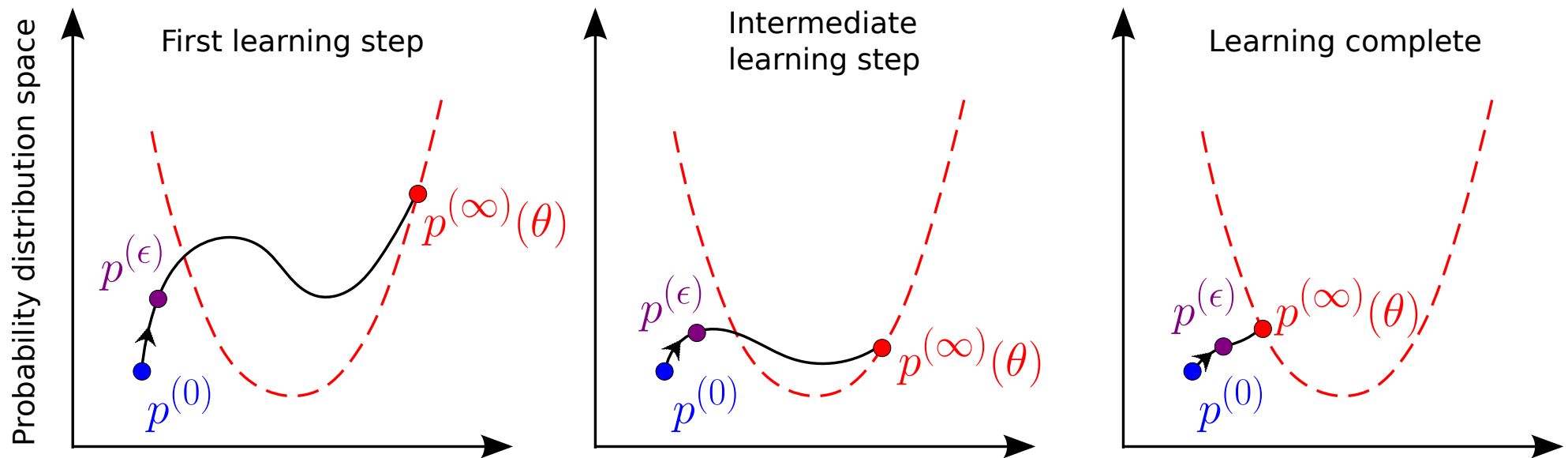


MPF Overview

- ...and only compare the data distribution to the distribution obtained by evolving the dynamics for a small time ϵ !



Minimum probability flow Overview



Master Equation

- Transition rates Γ_{ij}
- Master equation conserves probability

$$\dot{p}_i^{(t)} = \sum_{j \neq i} \Gamma_{ij}(\theta) p_j^{(t)} - \sum_{j \neq i} \Gamma_{ji}(\theta) p_i^{(t)}$$

flow into state i
from other states j

flow into other states j
from state i

- or in matrix form...:

$$\Gamma_{ii} := - \sum_{j \neq i} \Gamma_{ji}$$

$$\dot{\mathbf{p}}^{(t)} = \mathbf{\Gamma} \mathbf{p}^{(t)}$$

$$\mathbf{p}^{(t)} = \exp(\mathbf{\Gamma} t) \mathbf{p}^{(0)}$$

Detailed Balance

- Detailed balance

$$\Gamma_{ji} p_i^{(\infty)}(\theta) = \Gamma_{ij} p_j^{(\infty)}(\theta)$$

- Choose Γ to converge to model distribution

$$\frac{\Gamma_{ij}}{\Gamma_{ji}} = \frac{p_i^{(\infty)}(\theta)}{p_j^{(\infty)}(\theta)} = \exp [E_j(\theta) - E_i(\theta)]$$

$$\Gamma_{ij} = g_{ij} \exp \left[\frac{1}{2} (E_j(\theta) - E_i(\theta)) \right]$$

$$g_{ij} = g_{ji} = \begin{cases} 0 & \text{unconnected states} \\ 1 & \text{connected states} \end{cases}$$

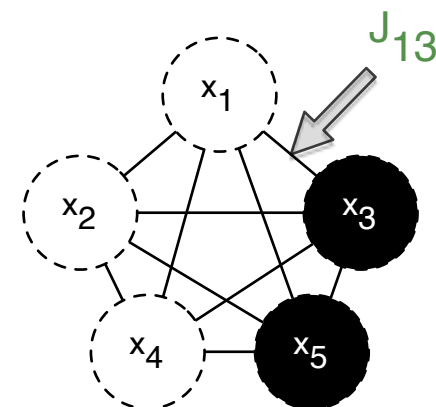
Demo Code

- 6 unit Ising model

$$p^{(\infty)}(\mathbf{x}; \mathbf{J}) = \frac{1}{Z(\mathbf{J})} \exp \left[- \sum_{i,j} J_{ij} x_i x_j \right]$$

$x_i \in \{0, 1\}$

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$



- 2 dimensional random projection of $p^{(t)}$
- $\mathbf{p}^{(0)}$ 150 samples using random \mathbf{J}
- $\mathbf{p}^{(\infty)}(\theta)$ initialized to another random \mathbf{J}

Objective Function

- Minimize $D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\epsilon)} (\theta) \right)$, for small ϵ

$$\hat{\theta} = \arg \min_{\theta} K_{MPF} (\theta)$$

$$\begin{aligned} K_{MPF} (\theta) = D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\epsilon)} (\theta) \right) &\approx D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(t)} (\theta) \right) \Big|_{t=0} + \epsilon \frac{\partial D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(t)} (\theta) \right)}{\partial t} \Big|_{t=0} \\ &= \epsilon \sum_{j \notin \text{data}} \dot{p}_j^{(0)} \\ &= \epsilon \sum_{i \notin \text{data}} \sum_{j \in \text{data}} g_{ij} \exp \left[\frac{1}{2} (E_j (\theta) - E_i (\theta)) \right] p_j^{(0)} \end{aligned}$$

- Minimize initial probability flow from data states to non-data states
- No sampling!

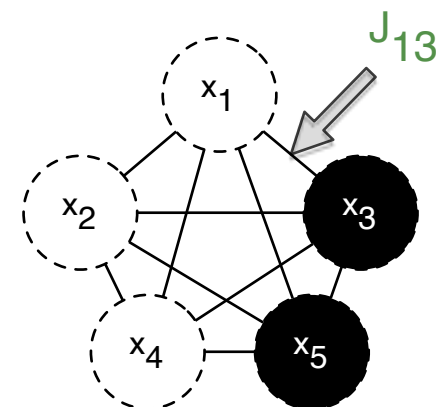
Demo Code

- 6 unit Ising model

$$p^{(\infty)}(\mathbf{x}; \mathbf{J}) = \frac{1}{Z(\mathbf{J})} \exp \left[- \sum_{i,j} J_{ij} x_i x_j \right]$$

$x_i \in \{0, 1\}$

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$



- 2 dimensional random projection of $\mathbf{p}^{(t)}$
- $\mathbf{p}^{(0)}$ 150 samples using random \mathbf{J}
- $\mathbf{p}^{(\infty)}(\theta)$ initialized to another random \mathbf{J}

Tractability

- Data distribution $p^{(0)}$ highly sparse
 - Ignore every column of Γ_{ij} for which $p_j^{(0)} = 0$
- Γ_{ij} is highly sparse
 - Each state connected to only a small number of other states (eg, within Hamming ball)
- Objective function evaluation costs $O(\text{number data points} \times \text{number connections per data point})$

$$K_{MPF}(\theta) = \epsilon \sum_{i \notin \text{data}} \sum_{j \in \text{data}} \Gamma_{ij} p_j^{(0)}$$

Contrastive Divergence

$$\Delta\theta_{CD} \propto - \sum_{i \notin \text{data}} \sum_{j \in \text{data}} p_j^{(0)} \left[\frac{\partial E_j(\theta)}{\partial \theta} - \frac{\partial E_i(\theta)}{\partial \theta} \right] \text{ [probability of MCMC step from } j \rightarrow i \text{]}$$

$$\frac{\partial K_{MPF}(\theta)}{\partial \theta} = \epsilon \sum_{i \notin \text{data}} \sum_{j \in \text{data}} p_j^{(0)} \left[\frac{\partial E_j(\theta)}{\partial \theta} - \frac{\partial E_i(\theta)}{\partial \theta} \right] g_{ij} \exp \left[\frac{1}{2} (E_j(\theta) - E_i(\theta)) \right]$$

- Markov Chain sampling/rejection step replaced by weighting factor
- Objective function!
- Unique global minima when model and data agree

Continuous State Spaces

- Analogous to sum \rightarrow integral transition

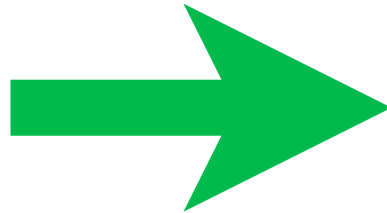
$$p_i^{(0)} = \begin{array}{l} \text{fraction data} \\ \mathcal{D} \text{ in state } i \end{array}$$

$$p^{(0)}(\mathbf{x}) = \frac{1}{\mathcal{D}} \sum_{\mathbf{x}_m \in \mathcal{D}} \delta(\mathbf{x} - \mathbf{x}_m)$$

$$p_i^{(t)}$$

$$p^{(t)}(\mathbf{x})$$

$$p_i^{(\infty)}(\theta) = \frac{\exp[-E_i(\theta)]}{Z(\theta)}$$



$$p^{(\infty)}(\mathbf{x}; \theta) = \frac{\exp[-E(\mathbf{x}; \theta)]}{Z(\theta)}$$

$$\Gamma_{ij} = g_{ij} \exp \left[\frac{1}{2} (E_j(\theta) - E_i(\theta)) \right]$$

$$\Gamma(\mathbf{x}_j \rightarrow \mathbf{x}_j) = g(\mathbf{x}_j \rightarrow \mathbf{x}_j) \exp \left[\frac{1}{2} (E(\mathbf{x}_j; \theta) - E(\mathbf{x}_i; \theta)) \right]$$

Score Matching

$$g(\mathbf{x}_j \rightarrow \mathbf{x}_i) = g(\mathbf{x}_i \rightarrow \mathbf{x}_j) = \begin{cases} 1 & \|\mathbf{x}_j - \mathbf{x}_i\|_2 < r \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} \lim_{r \rightarrow 0} K_{MPF} &\propto K_{SM} \\ &= \left\langle \frac{1}{2} \nabla_{\mathbf{x}} E(\mathbf{x}; \theta) \cdot \nabla_{\mathbf{x}} E(\mathbf{x}; \theta) - \nabla_{\mathbf{x}}^2 E(\mathbf{x}; \theta) \right\rangle_{p^{(0)}(\mathbf{x})} \end{aligned}$$

Objective Functions

- Maximum Likelihood

$$K_{ML} = D_{KL} \left(\mathbf{p}^{(0)} \parallel \mathbf{p}^{(\infty)}(\theta) \right)$$

- Minimum Probability flow

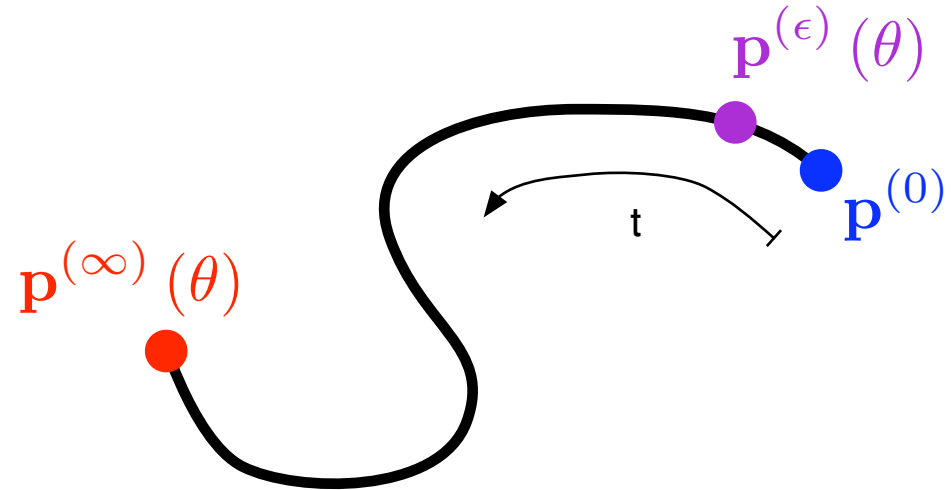
$$K_{MPF} = D_{KL} \left(\mathbf{p}^{(0)} \parallel \mathbf{p}^{(\epsilon)}(\theta) \right)$$

- Contrastive Divergence

$$K_{CD} \approx D_{KL} \left(\mathbf{p}^{(0)} \parallel \mathbf{p}^{(\infty)}(\theta) \right) - D_{KL} \left(\mathbf{p}^{(1)}(\theta) \parallel \mathbf{p}^{(\infty)}(\theta) \right)$$

- Score Matching

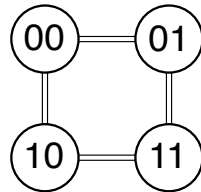
$$K_{SM} = \left\langle \frac{1}{2} \nabla_{\mathbf{x}} E(\mathbf{x}; \theta) \cdot \nabla_{\mathbf{x}} E(\mathbf{x}; \theta) - \nabla_{\mathbf{x}}^2 E(\mathbf{x}; \theta) \right\rangle_{p^{(0)}(\mathbf{x})}$$



Connectivity

- Discrete space
- Nearest neighbors

$$g_{ij} = g_{ji} = \begin{cases} 1 & i, j \text{ differ by 1 bit flip} \\ 0 & \text{otherwise} \end{cases}$$



Connectivity

- Continuous space
 - Hamiltonian dynamics (similar to hybrid Monte Carlo)
- Extend distribution to include auxiliary momentum variables \mathbf{q}

$$p^{(\infty)}(\mathbf{x}; \theta) \quad \rightarrow \quad p^{(\infty)}(\mathbf{x}, \mathbf{q}; \theta) = p^{(\infty)}(\mathbf{x}; \theta) p^{(\infty)}(\mathbf{q}) = \frac{e^{-H(\mathbf{x}, \mathbf{q}; \theta)}}{Z_H(\theta)}$$
$$H(\mathbf{x}, \mathbf{q}; \theta) = E(\mathbf{x}; \theta) + \frac{1}{2} \|\mathbf{q}\|_2^2$$

Connectivity

- Continuous space

$$p^{(\infty)}(\mathbf{x}; \theta) \xrightarrow{\text{green arrow}} p^{(\infty)}(\mathbf{x}, \mathbf{q}; \theta) = p^{(\infty)}(\mathbf{x}; \theta) p^{(\infty)}(\mathbf{q}) = \frac{e^{-H(\mathbf{x}, \mathbf{q}; \theta)}}{Z_H(\theta)}$$

$$H(\mathbf{x}, \mathbf{q}; \theta) = E(\mathbf{x}; \theta) + \frac{1}{2} \|\mathbf{q}\|_2^2$$

► Allow connectivity between momenta, and between states separated by leapfrog dynamics

$$\begin{aligned} g(\{\mathbf{x}_j, \mathbf{q}_j\} \rightarrow \{\mathbf{x}_i, \mathbf{q}_i\}) &= g(\{\mathbf{x}_i, \mathbf{q}_i\} \rightarrow \{\mathbf{x}_j, \mathbf{q}_j\}) \\ &= \begin{cases} 1 & \mathbf{x}_i = \mathbf{x}_j \\ 1 & \{\mathbf{x}_i, \mathbf{q}_i\} = \text{leapfrog}(\{\mathbf{x}_j, \mathbf{q}_j\}; \phi) \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

(transitions where only \mathbf{q} changes don't effect objective)

Connectivity

- Continuous space

$$p^{(\infty)}(\mathbf{x}; \theta) \xrightarrow{\quad} p^{(\infty)}(\mathbf{x}, \mathbf{q}; \theta) = p^{(\infty)}(\mathbf{x}; \theta) p^{(\infty)}(\mathbf{q}) = \frac{e^{-H(\mathbf{x}, \mathbf{q}; \theta)}}{Z_H(\theta)}$$
$$H(\mathbf{x}, \mathbf{q}; \theta) = E(\mathbf{x}; \theta) + \frac{1}{2} \|\mathbf{q}\|_2^2$$

$$\begin{aligned} g(\{\mathbf{x}_j, \mathbf{q}_j\} \rightarrow \{\mathbf{x}_i, \mathbf{q}_i\}) &= g(\{\mathbf{x}_i, \mathbf{q}_i\} \rightarrow \{\mathbf{x}_j, \mathbf{q}_j\}) \\ &= \begin{cases} 1 & \mathbf{x}_i = \mathbf{x}_j \\ 1 & \{\mathbf{x}_i, \mathbf{q}_i\} = \text{leapfrog}(\{\mathbf{x}_j, \mathbf{q}_j\}; \phi) \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

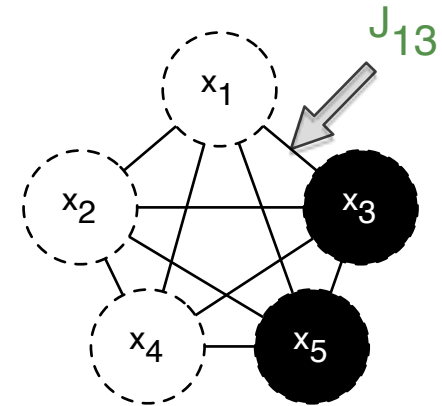
► Alternate between updating ϕ and minimizing K_{MPF}

1. Set $\phi = \theta$
2. Set $\theta = \arg \min_{\theta} K_{\text{MPF}}(\theta; \phi)$
3. Repeat

Examples - Ising

- Maximum entropy distribution over binary variables consistent with pairwise statistics

$$p^{(\infty)}(\mathbf{x}; \mathbf{J}) = \frac{1}{Z(\mathbf{J})} \exp \left[- \sum_{i,j} J_{ij} x_i x_j \right]$$
$$x_i \in \{0, 1\}$$
$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$



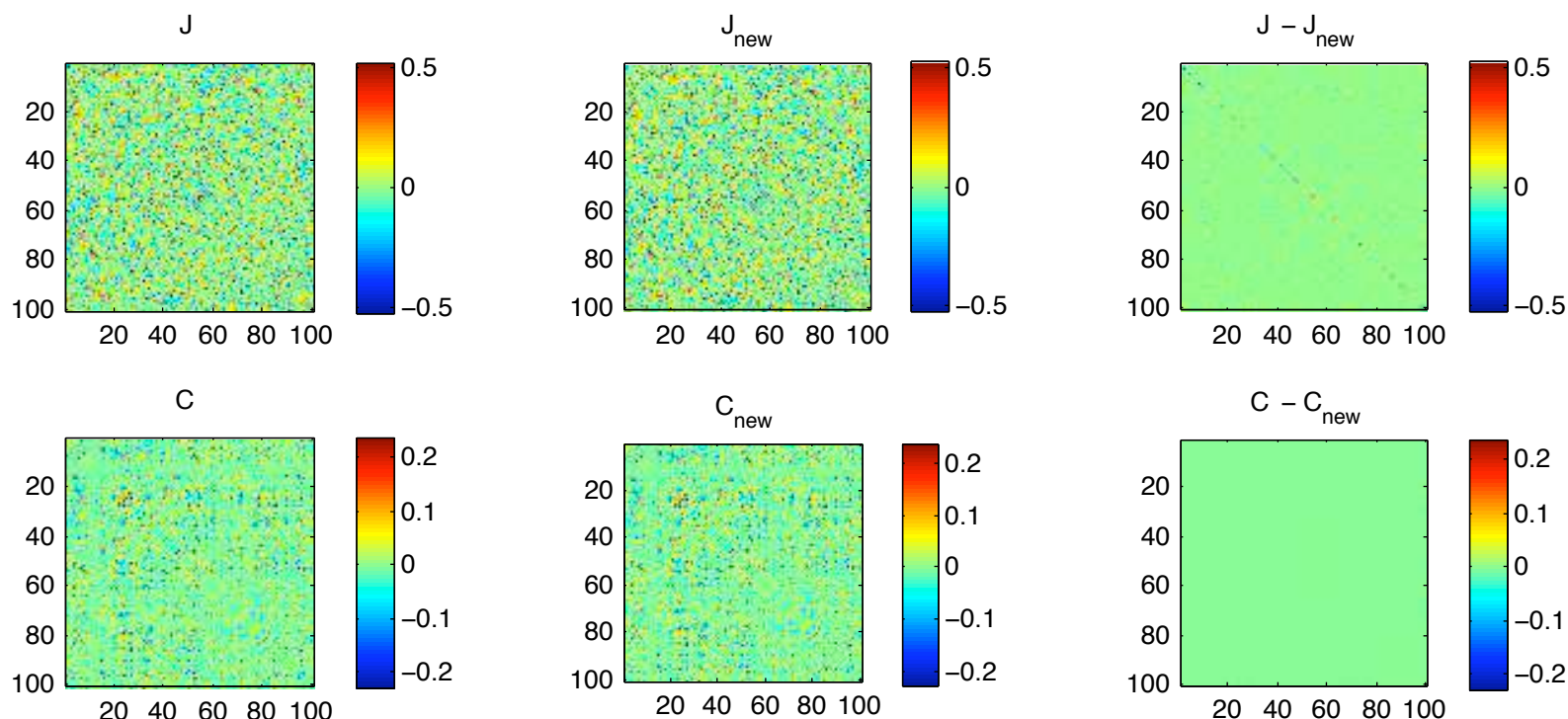
- > 2 orders of magnitude improvement in learning time

T Broderick, M Dudík, G Tkačik, R Schapire, and W Bialek. Faster solutions of the inverse pairwise ising problem. *E-print arXiv*, Jan 2007.

J Shlens, G D Field, J L Gauthier, M Greschner, A Sher, A M Litke, and E J Chichilnisky. The structure of large-scale synchronized firing in primate retina. *Journal of Neuroscience*, 29(15):5022–5031, Apr 2009.

Examples - Ising

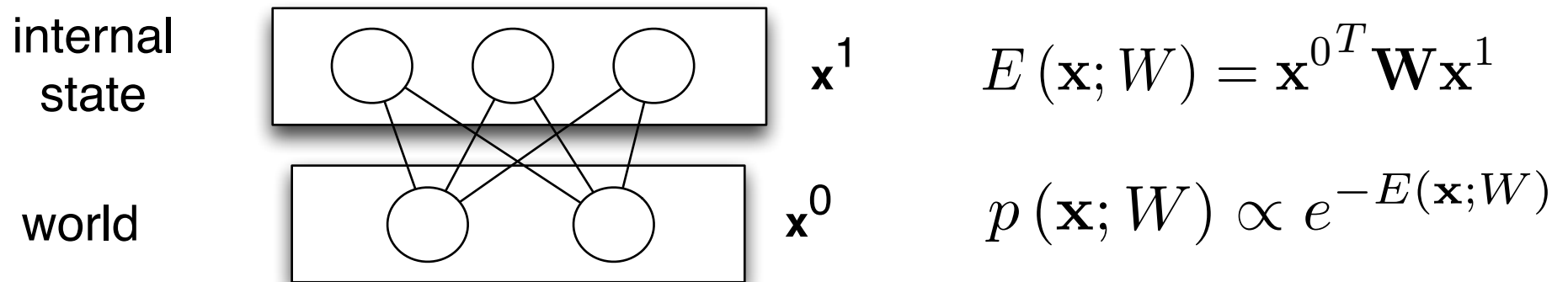
- MPF recovers Ising model parameters (100 units, 100,000 samples, J std. dev. 0.04)



$$p^{(\infty)}(\mathbf{x}; \mathbf{J}) = \frac{1}{Z(\mathbf{J})} \exp \left[- \sum_{i,j} J_{ij} x_i x_j \right] \quad x_i \in \{0, 1\}$$

Examples - RBM

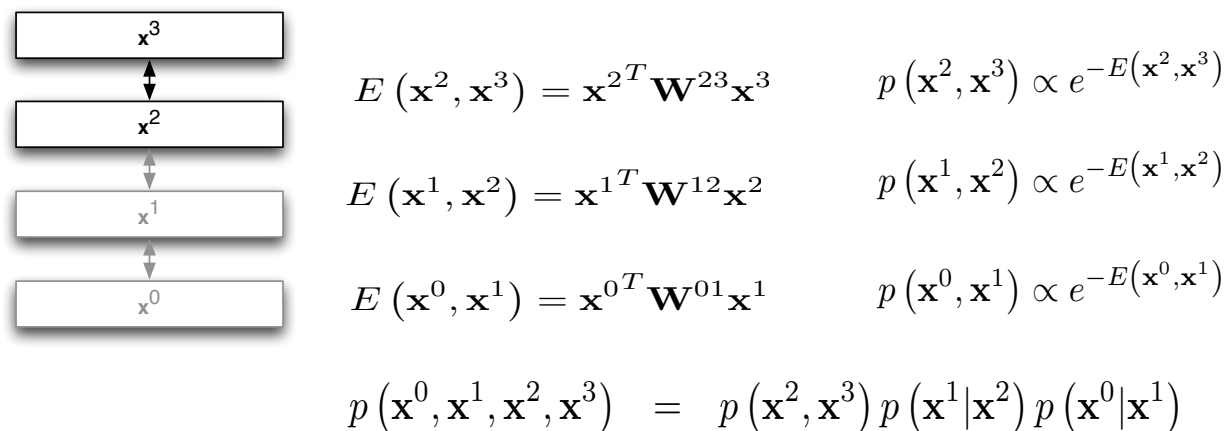
- Restricted Boltzmann Machine



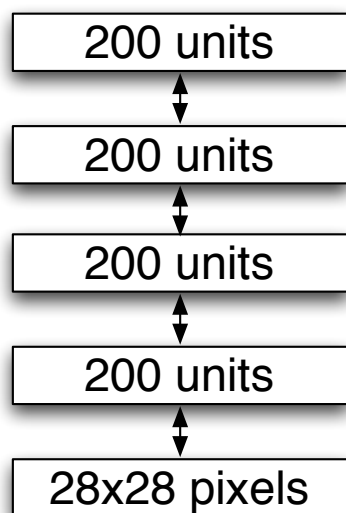
- Explicitly evaluate log likelihood on 20 visible unit, 20 hidden unit RBM
 - random -21.529931 bits
 - MPF -9.044596 bits
 - CDI -15.822924 bits
 - CDI0 -38.011133 bits (!!!) (continuing to increase!)

Examples - DBN

- Deep Belief Network is constructed by stacking RBMs

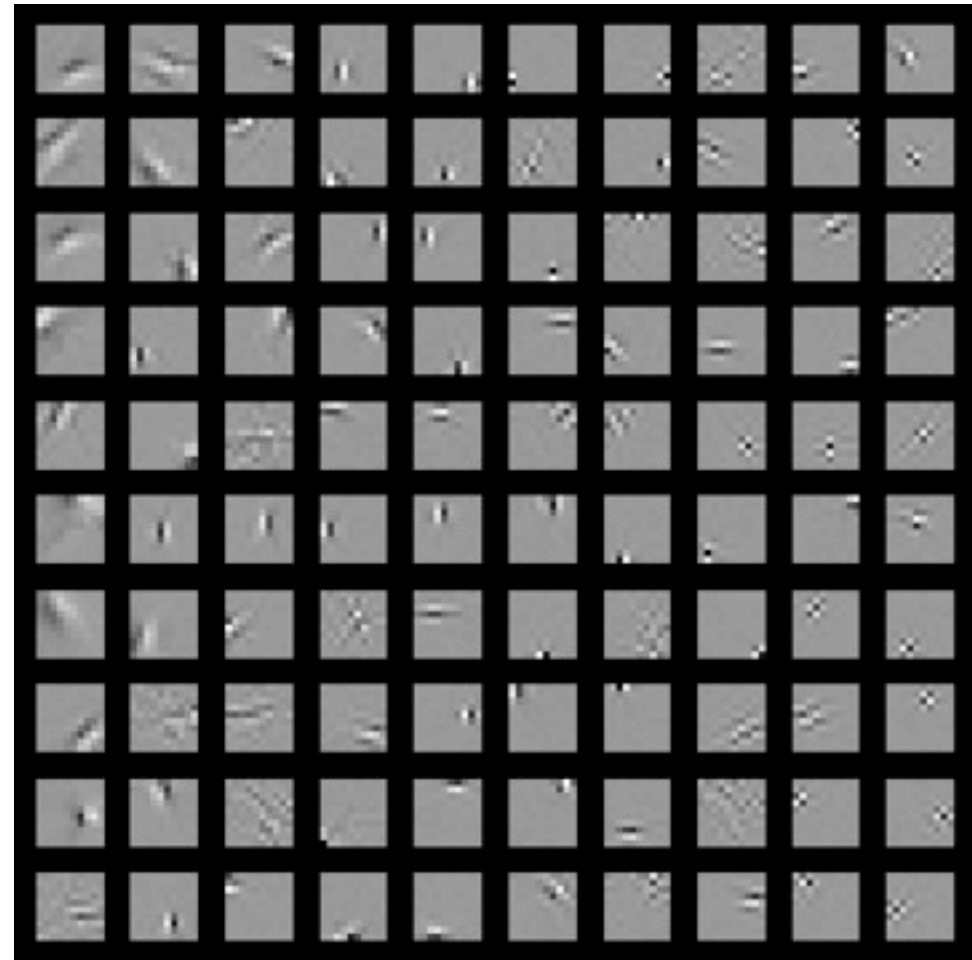
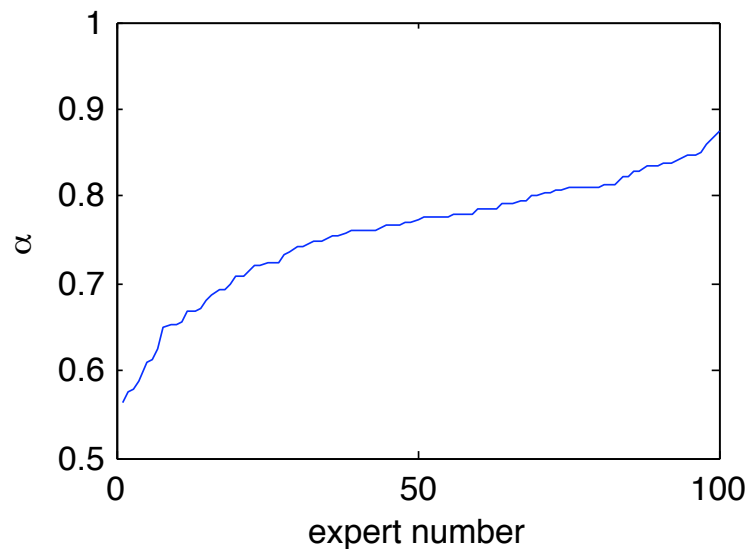


- Train DBN on MNIST digit database



Examples - Product of Student-t distributions

$$p^{(\infty)}(\mathbf{x}; \mathbf{J}, \alpha) \propto e^{-\sum_i \alpha_i \log[1 + (\mathbf{J}_i \mathbf{x})^2]}$$



MPF Summary

- General method for estimating parameters of probabilistic models
- Well defined objective function, which can be minimized using many known techniques (eg, l-BFGS, minFunc)
- Handles continuous and discrete systems
- Unique global minimum at Maximum Likelihood solution if model can exactly match data
- Convex for $\mathbf{E}(\theta)$ in exponential family (eg Ising model)
- Reduces to Minimum Velocity learning, Score Matching, and (certain forms of) Contrastive Divergence in appropriate limits

Thanks!

Co-authors



Peter Battaglini



Michael DeWeese

Discussion

Tony Bell
Yoshua Bengio
Charles Cadieu
Cristopher Hillar
Kilian Koepsell
Bruno Olshausen
Ashvin Vishwanath

Sharing results

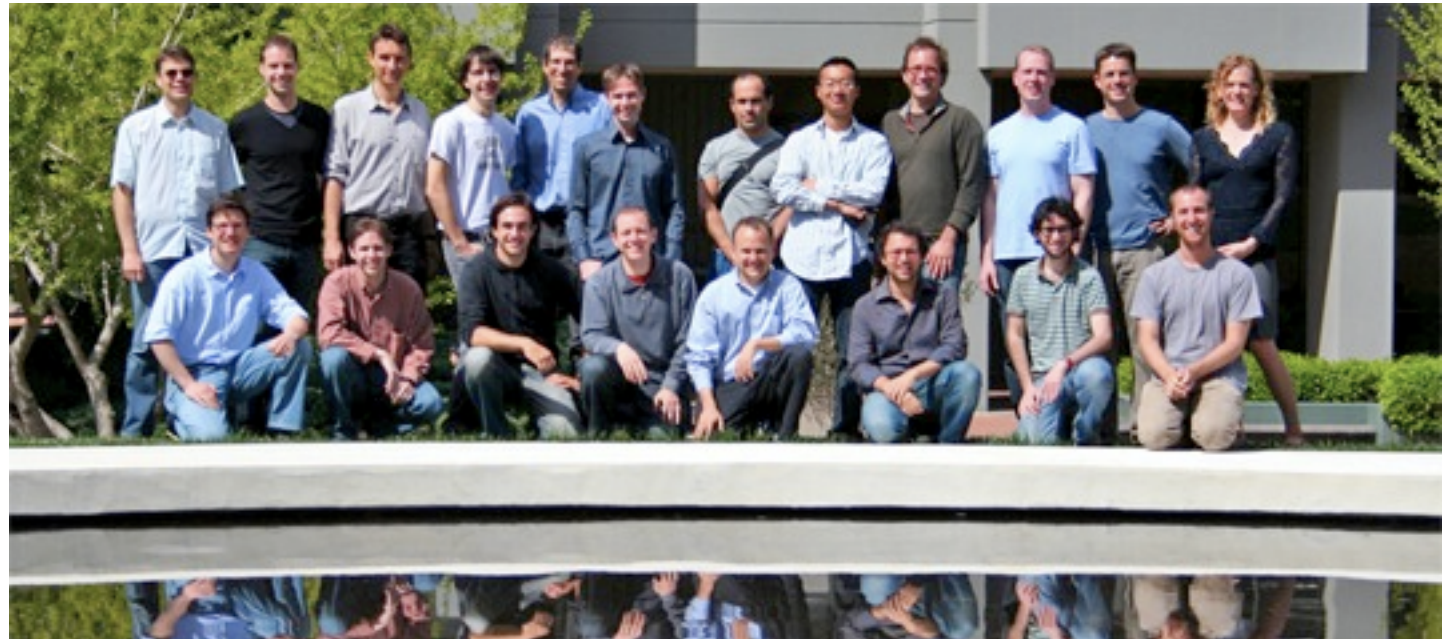
Javier Movellan
Jonathon Shlens
Tamara Broderick
Gasper Tcacik

Advisor



Bruno Olshausen

Redwood Center



Sampling Connectivity

$$\Gamma_{ji} p_i^{(\infty)}(\theta) = \Gamma_{ij} p_j^{(\infty)}(\theta) \qquad \langle \Gamma_{ji} \rangle = g_{ji} F_{ji}$$

$$\langle \Gamma_{ji} p_i^{(\infty)}(\theta) \rangle = \langle \Gamma_{ij} p_j^{(\infty)}(\theta) \rangle \qquad g_{ji} F_{ji} p_i^{(\infty)}(\theta) = g_{ij} F_{ij} p_j^{(\infty)}(\theta)$$

$$\langle \Gamma_{ji} \rangle p_i^{(\infty)}(\theta) = \langle \Gamma_{ij} \rangle p_j^{(\infty)}(\theta)$$

$$\frac{F_{ij}}{F_{ji}} = \frac{g_{ji} p_i^{(\infty)}(\theta)}{g_{ij} p_j^{(\infty)}(\theta)} = \frac{g_{ji}}{g_{ij}} \exp [E_j(\theta) - E_i(\theta)]$$

$$F_{ij} = \left(\frac{g_{ji}}{g_{ij}} \right)^{\frac{1}{2}} \exp \left[\frac{1}{2} (E_j(\theta) - E_i(\theta)) \right]$$

$$r_{ij} \sim \text{rand} [0, 1)$$

$$\Gamma_{ij} = \begin{cases} -\sum_{k \neq i} \Gamma_{ki} & i = j \\ F_{ij} & r_{ij} \leq g_{ij} \text{ and } i \neq j \\ 0 & r_{ij} > g_{ij} \text{ and } i \neq j \end{cases}$$

Examples - Power series

- Fitting a highly unstructured 2-dimensional distribution

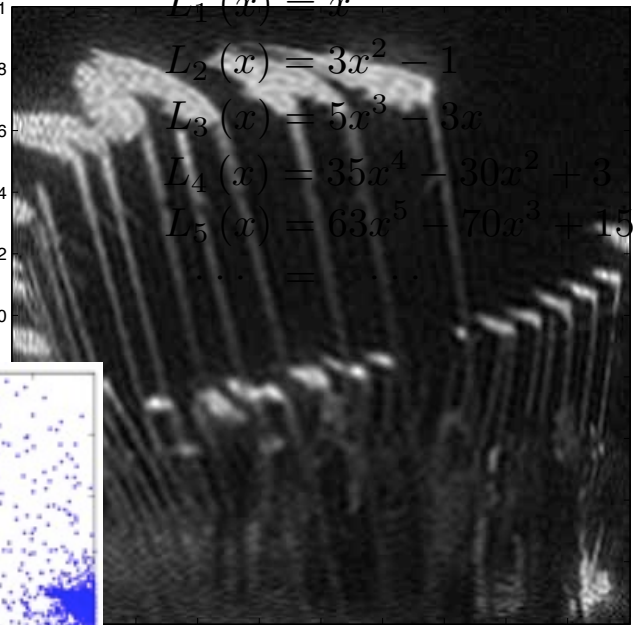
$$p^{(\infty)}(x, y; \theta) = \frac{1}{Z(\theta)} \exp \left[- \sum_{m,n=0}^M \theta_{mn} L_m(x) L_n(y) \right]$$



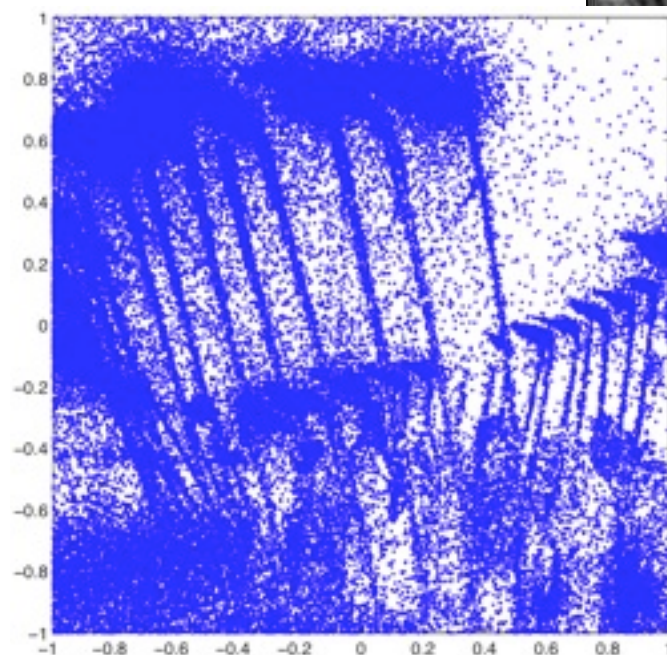
-0.4 -0.2 0 0.2 0.4 0.6 0.8 1

1]²

$$\begin{aligned} L_0(x) &= 1 \\ L_1(x) &= x \\ L_2(x) &= 3x^2 - 1 \\ L_3(x) &= 5x^3 - 3x \\ L_4(x) &= 35x^4 - 30x^2 + 3 \\ L_5(x) &= 63x^5 - 70x^3 + 15x \\ &\vdots = \vdots \end{aligned}$$



-0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1



scatterplot, 100,000 samples

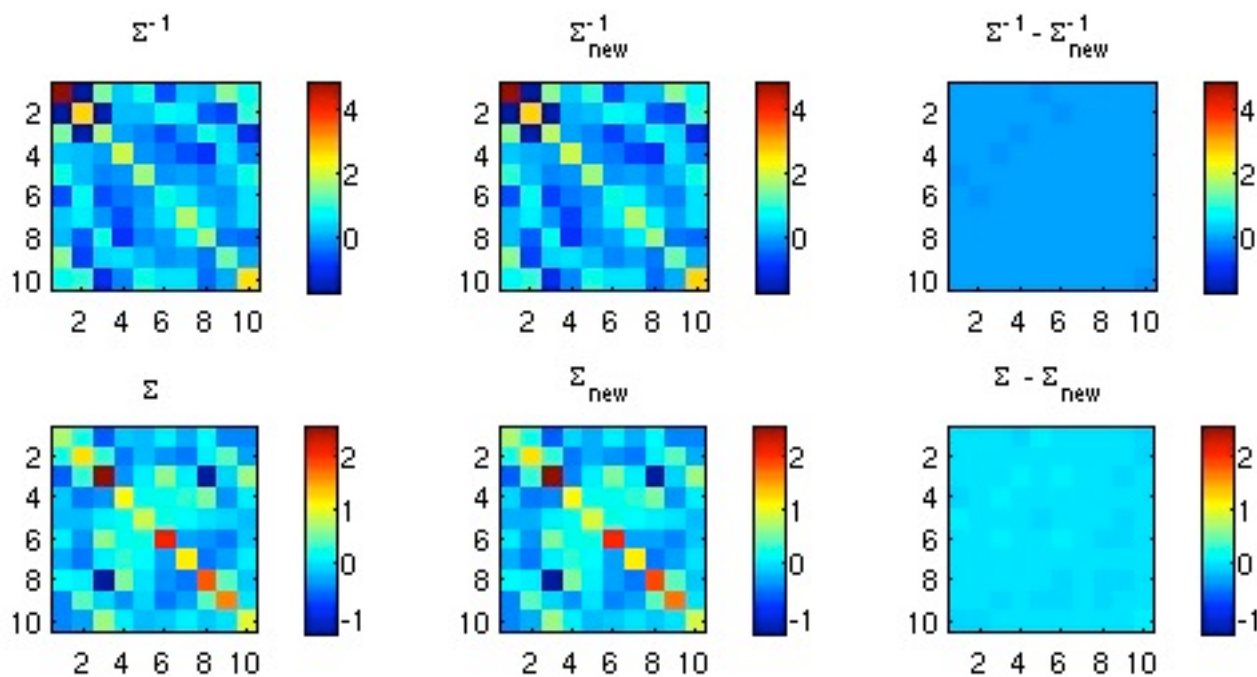
data histogram

model histogram

Examples - Gaussian

- MPF recovers parameters from 10,000 samples of a 10-dimensional Gaussian distribution

$$p^{(\infty)}(\mathbf{x}; \Sigma^{-1}) = \frac{1}{Z(\Sigma^{-1})} \exp \left[-\frac{1}{2} \mathbf{x}^T \Sigma^{-1} \mathbf{x} \right]$$



Relationship to CD

$$K_{CD} \approx D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\infty)}(\theta) \right) - D_{KL} \left(\mathbf{p}^{(\epsilon)}(\theta) || \mathbf{p}^{(\infty)}(\theta) \right)$$

$$K_{MPF} = D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\epsilon)}(\theta) \right)$$

$$D_{KL} (A||C) \leq D_{KL} (A||B) + D_{KL} (B||C)$$

$$D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\infty)}(\theta) \right) \leq D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\epsilon)}(\theta) \right) + D_{KL} \left(\mathbf{p}^{(\epsilon)}(\theta) || \mathbf{p}^{(\infty)}(\theta) \right)$$

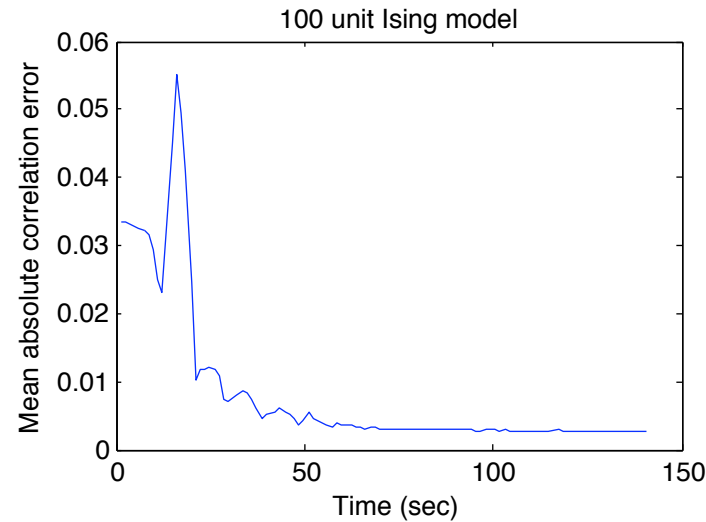
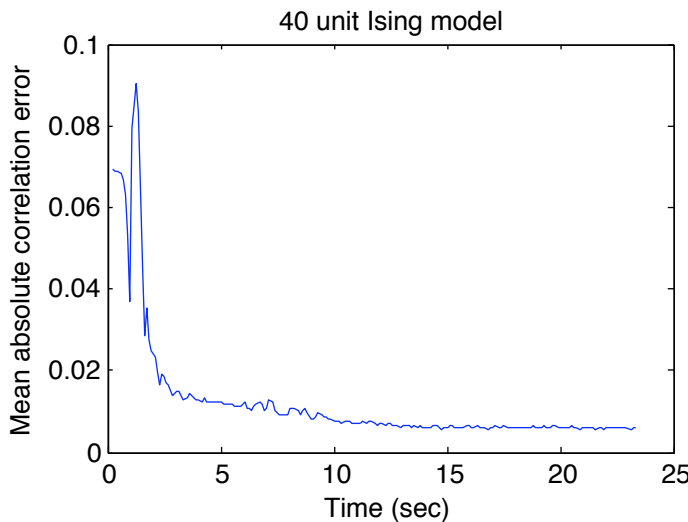
$$D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\infty)}(\theta) \right) - D_{KL} \left(\mathbf{p}^{(\epsilon)}(\theta) || \mathbf{p}^{(\infty)}(\theta) \right) \leq D_{KL} \left(\mathbf{p}^{(0)} || \mathbf{p}^{(\epsilon)}(\theta) \right)$$

$$K_{CD} \leq K_{MPF}$$

Examples - Ising

T Broderick, M Dudík, G Tkačik, R Schapire, and W Bialek. Faster solutions of the inverse pairwise ising problem. *E-print arXiv*, Jan 2007.

- Takes Broderick et al ~200 seconds on ~100 cores to recover parameters for 40 unit Ising model from 20,000 samples
- Using their J matrix, takes MPF ~15 seconds on 8 cores

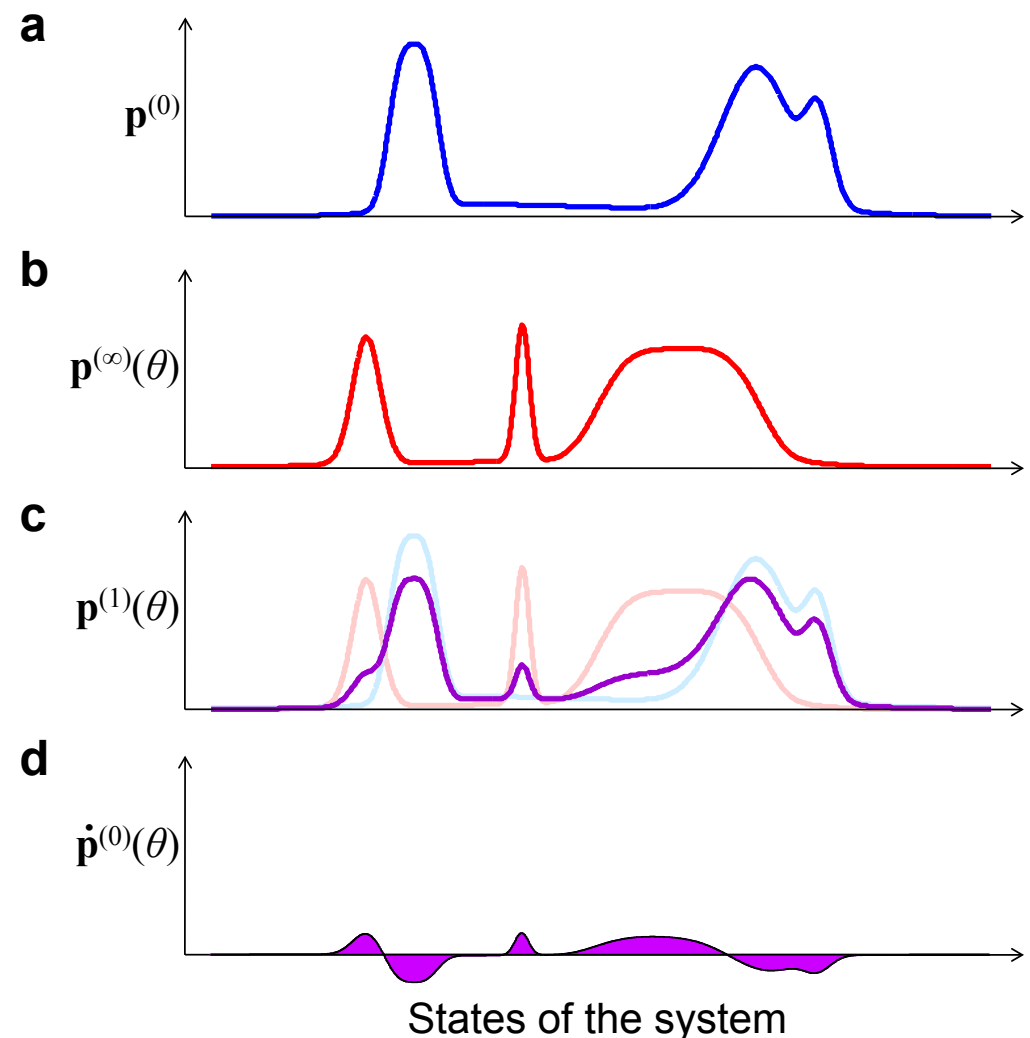


- Learning is ~ 2 orders of magnitude faster

Objective function

Alternate interpretation

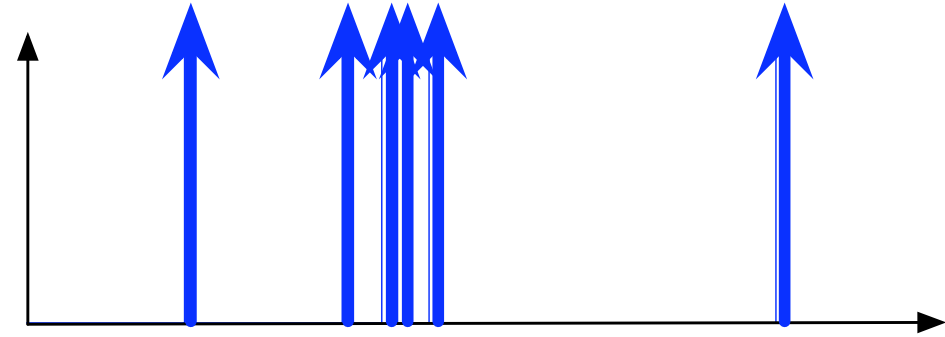
- Dynamics turn data distribution (a) into model distribution (b)
- (c) shows distribution at intermediate time
- The objective is to minimize the initial flow of probability away from the data, the shaded area in (d).



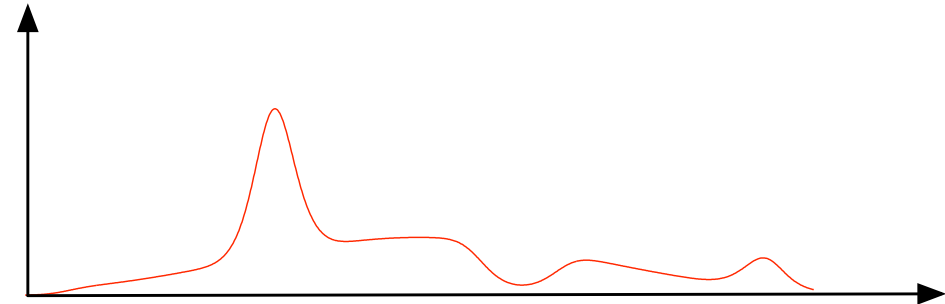
Alternative view

- Dynamics turn data distribution into model distribution
- Objective is to minimize initial flow of probability away from data - the shaded area

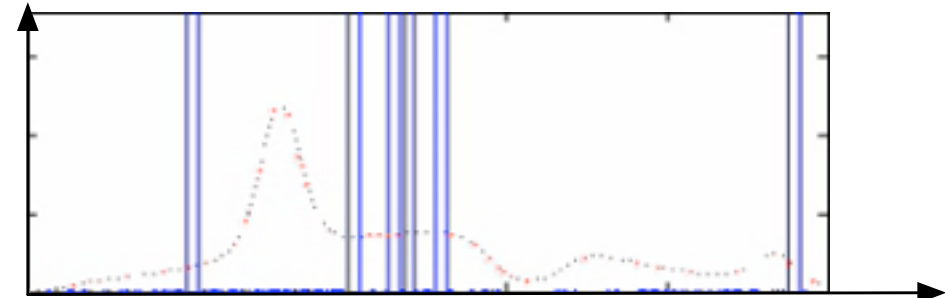
$$p^{(0)}$$



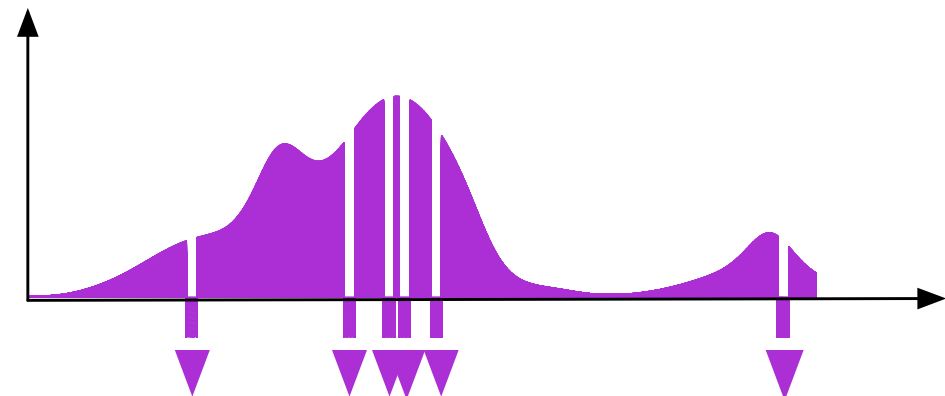
$$p^{(\infty)}(\theta)$$



$$p^{(t)}(\theta)$$

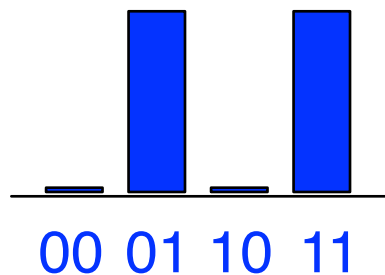


$$\dot{p}^{(0)}(\theta)$$



States of the System

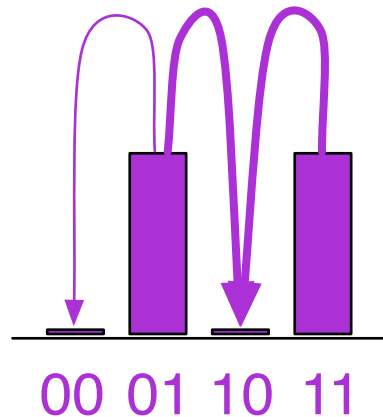
MPF - Dynamics



data distribution

$$p_i^{(0)} = \text{data}$$

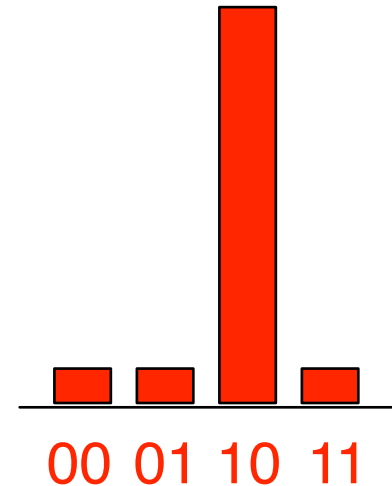
$$\dot{p}_i^{(0)} = \sum_j \Gamma_{ij}(\theta) p_j^{(0)}$$



dynamics



$$\dot{p}_i^{(t)} = \sum_j \Gamma_{ij}(\theta) p_j^{(t)}(\theta)$$



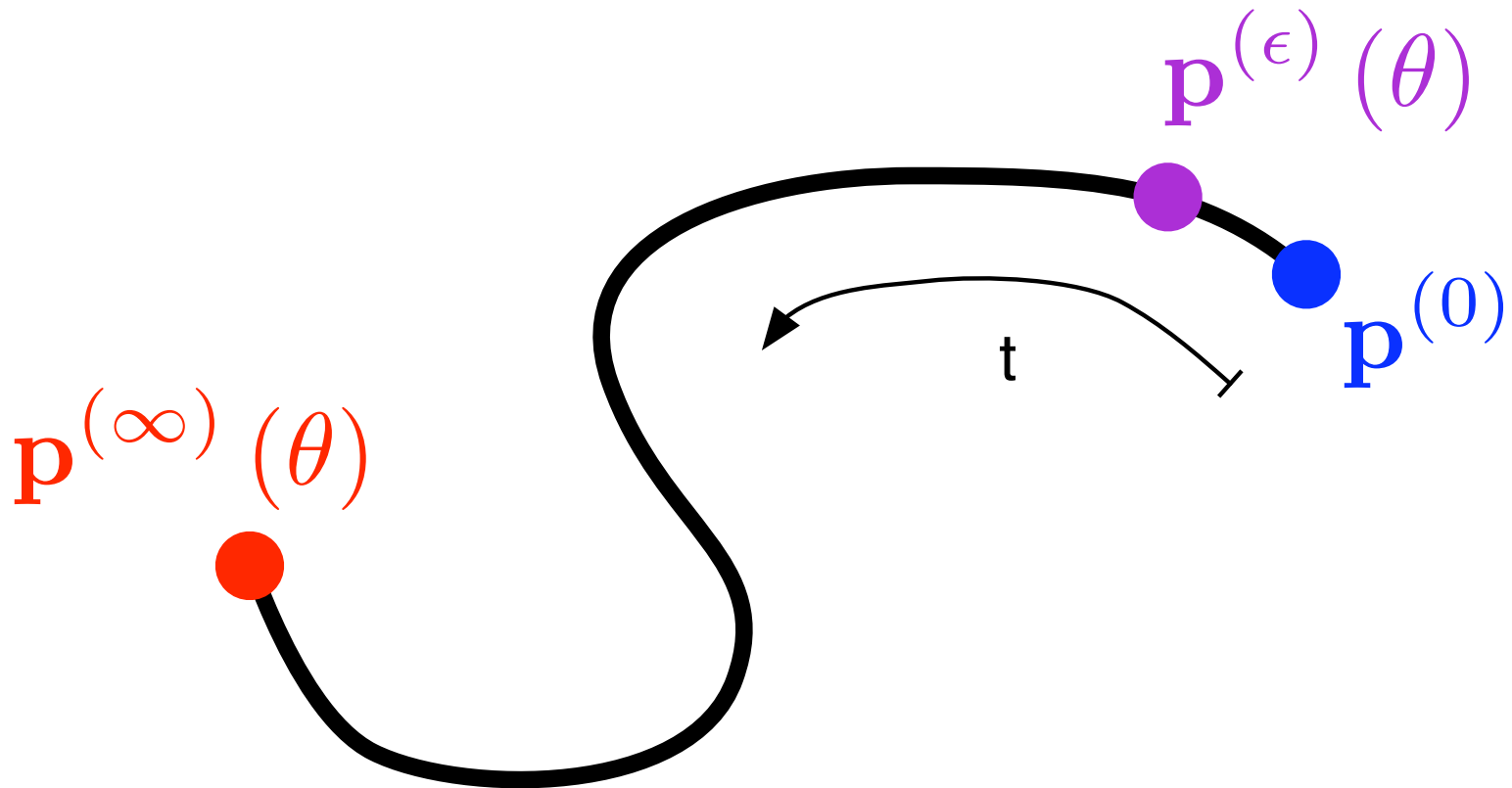
model distribution

$$p_i^{(\infty)}(\theta) = \frac{e^{-E_i(\theta)}}{Z(\theta)}$$

$$\dot{p}_i^{(\infty)} = 0$$

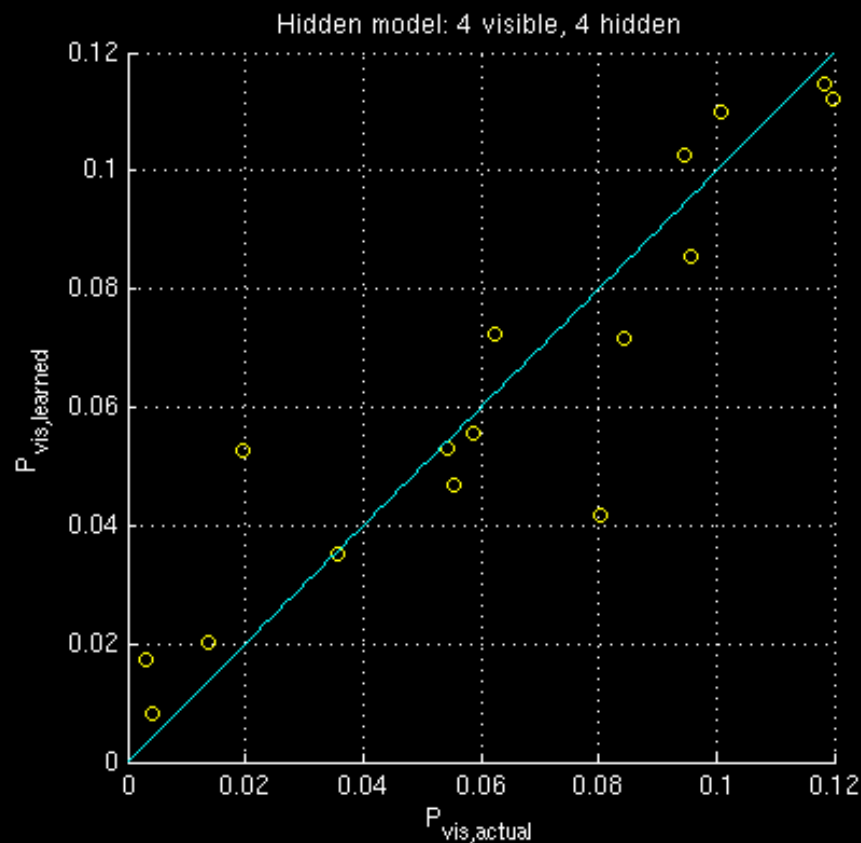
- Most Monte Carlo methods implement a stochastic version of these dynamics

Minimum probability flow Overview

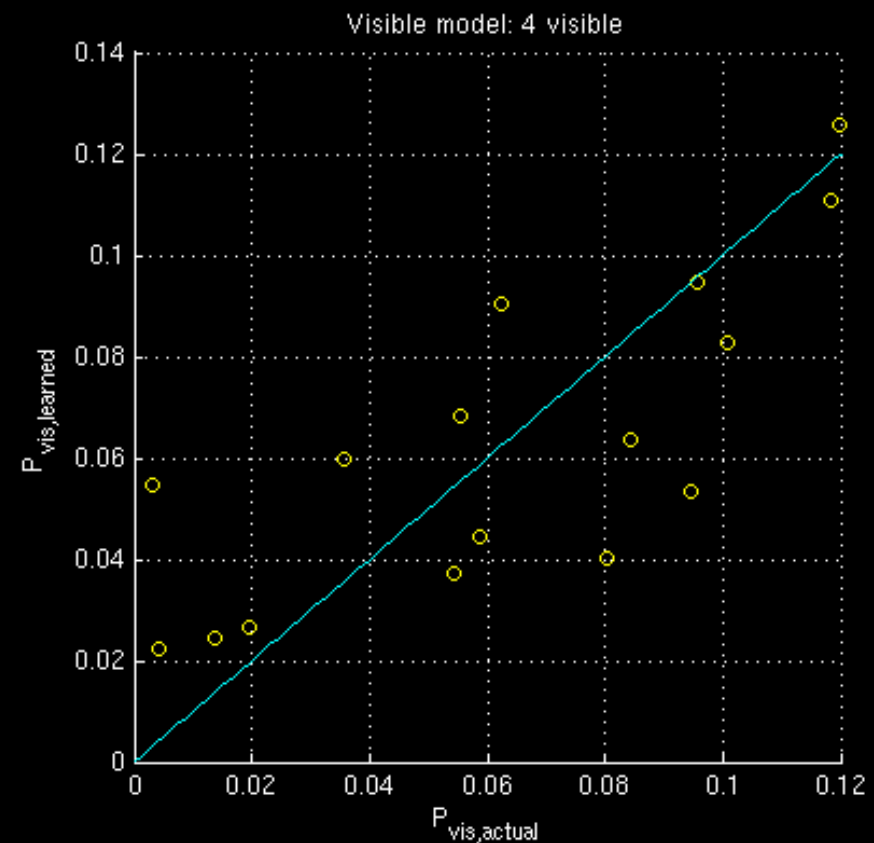


Example: Boltzmann Machine

Comparison of actual visible state probabilities:
4 visible, 4 hidden VS. only 4 visible



Hidden model



Visible model