Select and Sample – A model of efficient neural inference and learning

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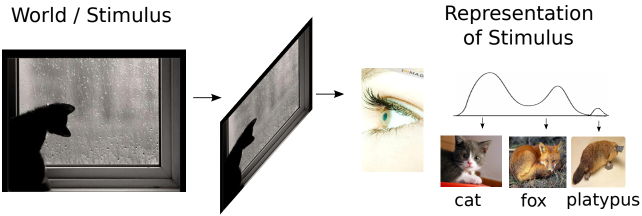
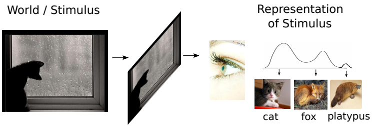
Introduction



- **Experimental neuroscience evidence**: perception encodes and maintains posterior probability distributions over possible causes of sensory stimuli
- Most likely stimulus interpretation(s) + associated uncertainty

Introduction - Motivation



- Full posterior representation costly/complex – very high-dimensional, multi-modal, possibly highly correlated
- But, the brain can nevertheless perform rapid learning and inference
- Evidence for fast feed-forward processing and recurrent processing

Questions:

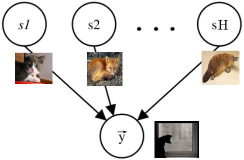
- Can we find rich representation of the posterior for very high-dimensional spaces?
- This goal believed to be shared by the brain, can find a biologically plausible solution reaching it?

Goals:

- Want: method to combine feed-forward processing and recurrent stages of processing
- Idea: formulate these 2 ideas as approximations to exact inference in a probabalistic framework

The Setting

- Probabalistic generative model with
  latent causes/obj $\vec{s} = (s_1, \ldots, s_H)$ for

  sensory data $\vec{y} = (y_1, \ldots, y_D)$,

  and parameters Θ:

$$p(\vec{y} \,|\, \Theta) = \sum_{\vec{s}} p(\vec{y} \,|\, \vec{s}, \Theta)\, p(\vec{s} \,|\, \Theta)$$

- Optimization problem: given data set $Y = \{\vec{y}_1, \ldots, \vec{y}_N\}$ find maximum likelihood parameters Θ^*:

$$\Theta^* = \underset{\Theta}{\operatorname{argmax}}\; p(Y \,|\, \Theta)$$

  using expectation maximization (EM).

The Setting - Expectation Maximization (EM)

Maximize objective function $\mathcal{L}(\Theta) = \log p(\,Y\,|\,\Theta)$ w.r.t. Θ by optimizing a lower bound, the *free-energy*,

$$\mathcal{L}(\Theta) \geq \mathcal{F}(\Theta, q) = \sum_{s} q(\vec{s}|\Theta) \log \frac{p(\vec{y}, \vec{s}|\Theta)}{p(\vec{s}|\Theta)}$$
$$= \langle \log p(\vec{y}, \vec{s}) \rangle_{q(\vec{s}|\Theta)} + \mathsf{H}[q(\vec{s})]$$

...using EM: iteratively optimize $\mathcal{F}(\Theta, q)$,

E-step: estimate posterior distribution q, parameters fixed

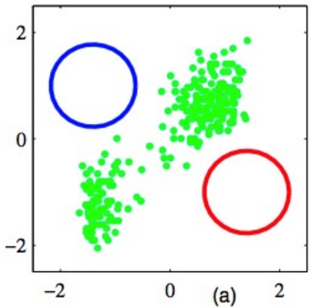
$$\underset{q(\vec{s}|\Theta)}{\operatorname{argmax}} \mathcal{F}(\Theta, q) \rightarrow q_n(\vec{s}|\Theta) := p(\vec{s}^{(n)}\,|\,\vec{y}^{(n)}, \Theta)$$

M-step: estimate model parameters, q fixed

$$\underset{\Theta}{\operatorname{argmax}} \mathcal{F}(\Theta, q) \rightarrow \Theta := \underset{\Theta}{\operatorname{argmax}} \langle \log p(\vec{y}, \vec{s}) \rangle_{q(\vec{s}|\Theta)}$$

The Setting - EM example

Mixture of Gaussians: using EM iteratively optimize $\mathcal{F}(\Theta, q)$:

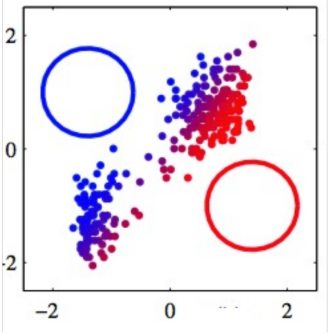


(a)

Task: cluster data into 2 classes/Gaussians $\rightarrow$ Initialize parameters randomly before iterating E- and M-steps

The Setting - EM example

Mixture of Gaussians: using EM iteratively optimize $\mathcal{F}(\Theta, q)$:



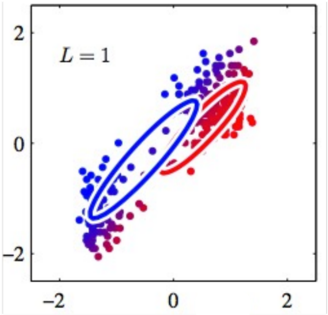
Iteration 1:

E-step: estimate posterior distribution q, parameters fixed

$$\operatorname*{argmax}_{q(\vec{s}|\Theta)} \mathcal{F}(\Theta, q) \to q_n(\vec{s}|\Theta) := p(\vec{s}^{(n)}|\vec{y}^{(n)}, \Theta)$$

The Setting - EM example

Mixture of Gaussians: using EM iteratively optimize $\mathcal{F}(\Theta, q)$:



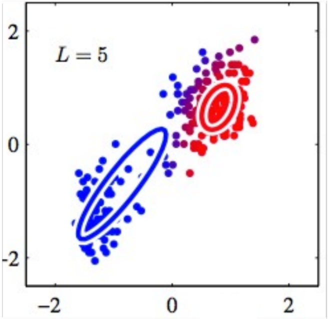
Iteration 1:

M-step: estimate model parameters, q fixed

$$\underset{\Theta}{\operatorname{argmax}}\, \mathcal{F}(\Theta, q) \rightarrow \Theta := \underset{\Theta}{\operatorname{argmax}} \langle \log p(\vec{y}, \vec{s}) \rangle_{q(\vec{s}|\Theta)}$$

The Setting - EM example

Mixture of Gaussians: using EM iteratively optimize $\mathcal{F}(\Theta, q)$:



Iteration 5:

E-step: estimate posterior distribution q, parameters fixed

$$\underset{q(\vec{s}|\Theta)}{\operatorname{argmax}} \mathcal{F}(\Theta, q) \rightarrow q_n(\vec{s}|\Theta) := p(\vec{s}^{(n)}|\vec{y}^{(n)}, \Theta)$$

M-step: estimate model parameters, q fixed

$$\underset{\Theta}{\operatorname{argmax}} \mathcal{F}(\Theta, q) \rightarrow \Theta := \underset{\Theta}{\operatorname{argmax}} \langle \log p(\vec{y}, \vec{s}) \rangle_{q(\vec{s}|\Theta)}$$

The Setting - Costly bit of EM

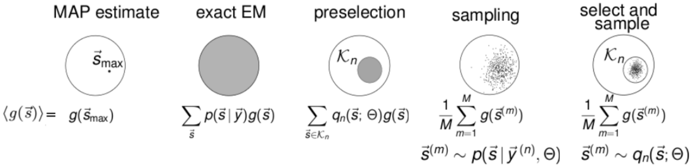
- M-step usually involves a small number of expected values w.r.t. the posterior distribution:

$$\langle g(\vec{s}) \rangle_{p(\vec{s}\,|\,\vec{y}^{\,(n)},\Theta)} = \sum_{\vec{s}} p(\vec{s}\,|\,\vec{y}^{\,(n)},\Theta)\, g(\vec{s})$$

  where $g(\vec{s})$ e.g. elementary function of hidden variables – $g(\vec{s}) = \vec{s}$ or $g(\vec{s}) = \vec{s}\vec{s}^T$ for standard sparse coding

- Computation of expectations is usually the computationally demanding part

Approach: Select and Sample

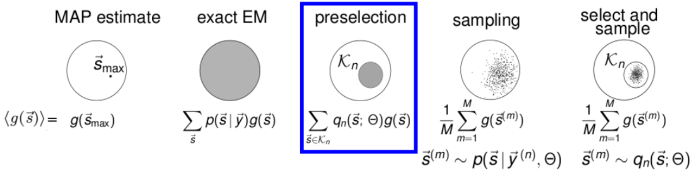


Method of attack: approximate expectation values in 2 ways

- **1. Selection** $\approx$ feed-forward processing: Restrict approximate posterior to pre-selected states:

- **2. Sampling** $\approx$ recurrent processing: approximate expectations using samples from the posterior distribution in a Monte Carlo estimate of expectations

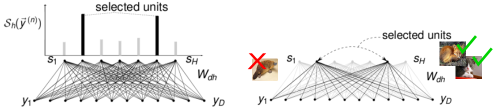
Approach: Select and Sample



- **1. Selection** $\approx$ feed-fwd: Restrict approximate posterior to pre-selected states:

$$p(\vec{s} \,|\, \vec{y}^{\,(n)}, \Theta) \approx q_n(\vec{s}; \Theta) = \frac{p(\vec{s} \,|\, \vec{y}^{\,(n)}, \Theta)}{\sum_{\vec{s}\,' \in \mathcal{K}_n} p(\vec{s}\,' \,|\, \vec{y}^{\,(n)}, \Theta)} \, \delta(\vec{s} \in \mathcal{K}_n)$$

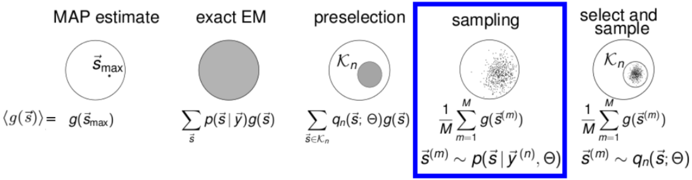
- Choose set $\mathcal{K}_n$ w/ *selection function* $\mathcal{S}_h(\vec{y}, \Theta)$; efficiently selects candidates s_h with most posterior mass:



- Efficiently compute expectations in $\mathcal{O}(|\mathcal{K}_n|)$:

$$\langle g(\vec{s}) \rangle_{p(\vec{s} \,|\, \vec{y}^{\,(n)}, \Theta)} \approx \langle g(\vec{s}) \rangle_{q_n(\vec{s}; \Theta)} = \frac{\sum_{\vec{s} \in \mathcal{K}_n} p(\vec{s}, \vec{y}^{\,(n)} \,|\, \Theta) \, g(\vec{s})}{\sum_{\vec{s}\,' \in \mathcal{K}_n} p(\vec{s}\,', \vec{y}^{\,(n)} \,|\, \Theta)}$$

Approach: Select and Sample



Method of attack: approximate expectation values in 2 ways

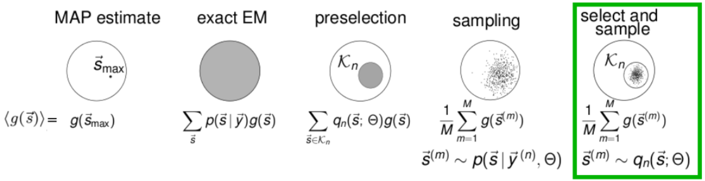
- **2. Sampling** $\approx$ recurrent processing: approximate expectations using samples from the posterior distribution in a Monte Carlo estimate:

$$\langle g(\vec{s}) \rangle_{p(\vec{s} \,|\, \vec{y}^{(n)}, \Theta)} \approx \frac{1}{M} \sum_{m=1}^{M} g(\vec{s}^{(m)})$$

with $\vec{s}^{(m)} \sim p(\vec{s} \,|\, \vec{y}, \Theta)$

- Obtaining samples from true posterior often difficult

Approach: Select and Sample



Method of attack: approximate expectation values in 2 ways

- **Combine Selection + Sampling**: approx. using samples from the **truncated distribution**:

$$\langle g(\vec{s})\rangle_{p(\vec{s}\,|\,\vec{y}^{(n)},\Theta)} \approx \frac{1}{M}\sum_{m=1}^{M} g(\vec{s}^{(m)})$$

with $\vec{s}^{(m)} \sim q_n(\vec{s};\Theta)$

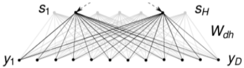
- Subspace $\mathcal{K}_n$ is small, allowing MCMC algorithms to operate more efficiently, i.e. shorter burn-in times, reduced number of required samples

Example application - Binary sparse coding

Apply select and sample - sparse coding model with binary latents:

$$p(\vec{s}|\pi) \quad = \quad \prod_{h=1}^{H} \pi^{s_h} \big(1-\pi\big)^{1-s_h}$$

$$p(\vec{y}|\vec{s}, W, \sigma) \quad = \quad \mathcal{N}(\vec{y};\, W\vec{s}, \sigma^2 I)$$



$\vec{y} \in \mathbb{R}^D$	observed variables	π	prior parameter
$\vec{s} \in \{0,1\}^H$	hidden variables	σ	noise level
$W \in \mathbb{R}^{D\times H}$	dictionary		

$$p(\vec{y}\,|\,\Theta) = \sum_{s} \mathcal{N}(\vec{y};\, W\vec{s}, \sigma^2 I) \prod_{h=1}^{H} \pi^{s_h} \big(1-\pi\big)^{1-s_h}$$

Selection function: cosine similarity - take H' highest scored s_h with:

$$\mathcal{S}_h(\vec{y}^{\,(n)}) = \frac{\vec{W}_h^{\mathrm{T}} \vec{y}^{\,(n)}}{\|\,\vec{W}_h\|}$$

Example application - Binary sparse coding

- Inference: selection + Gibbs sampling; selection posterior equivalent to full post. with only selected dims

$$p(s_h = 1 \mid \vec{s}_{\backslash h}, \vec{y}) = \frac{p(s_h = 1, \vec{s}_{\backslash h}, \vec{y})^\beta}{p(s_h = 0, \vec{s}_{\backslash h}, \vec{y})^\beta + p(s_h = 1, \vec{s}_{\backslash h}, \vec{y})^\beta}$$

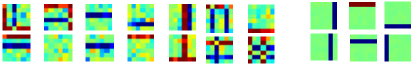
- Complexity of E-step (all 4 BSC cases):

$$\mathcal{O}\Big(N S(\underbrace{D}_{p(\vec{s},\vec{y})} + \underbrace{1}_{\langle \vec{s} \rangle} + \underbrace{H}_{\langle \vec{s}\vec{s}^T \rangle})\Big)$$

where S is # of evaluated hidden states

Experiments - 1. Artificial data

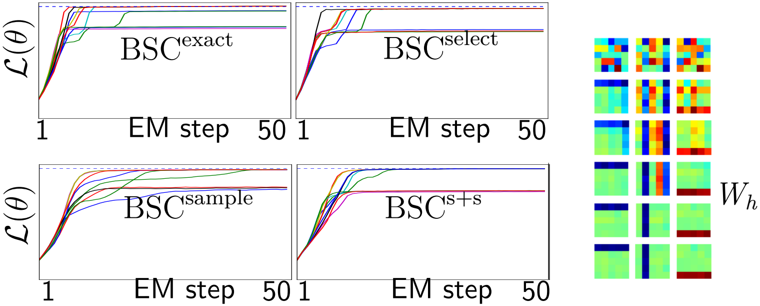
- Goal: observe convergence behavior; sanity check for our method with ground-truth
- Data: $N = 2000$ bars data consisting of $D = 6 \times 6 = 36$ pixels with $H = 12$ bars: $\vec{y}^{(n)}$ W_h



- Experiments: binary sparse coding with:
  (1) exact inference, (2) selection alone,
  (3) sampling alone, (4) selection + sampling

Experiments – 1. Artificial data

Convergence behavior of 4 methods

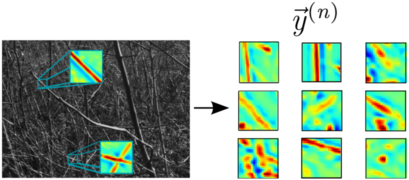


- Shown: dotted line / $\mathcal{L}(\theta^{ground-truth})$, dictionary elements W_h, and log-likelihood for multiple runs over 50 EM steps for all 4 methods

$\rightarrow$ select and sample extracts GT parameters; likelihood converges

Experiments - 2. Natural image patches

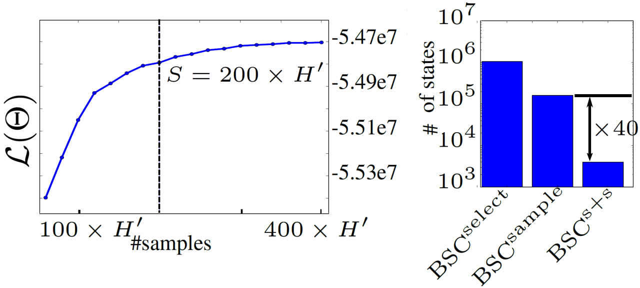
- Goals: [1] detirmine reasonable # of samples, performance of select and sample for H' range
  [2] compare # states each method must evaluate
- Data: $N = 40,000$ image patches with $D = 26 \times 26 = 676$ pixels, with $H = 800$ hidden dimensions:



- Experiments: binary sparse coding with $12 \leq H' \leq 36$ for all inference methods:
  (1) selection alone, (2) sampling alone,
  (3) selection + sampling

Experiments – 2. Natural image patches

Evaluation of select and sample approach



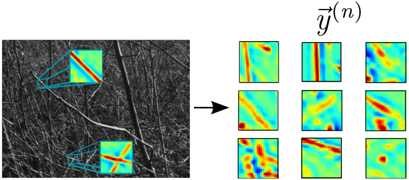
- Shown: end approx. log-likelihood after 100 EM-steps vs. # samples per data point and # states must evaluate for $H' = 20$

$\rightarrow$ 200 samples/hid dimension sufficient: $\leq 1\%$ likelihood increase

$\rightarrow$ Select and sample – $\times 40$ faster than sampling

Experiments – 3. Large scale on image patches

- Goals: large scale using # of samples detirmined in exp 2
- Data: $N = 500,000$ image patches $D = 40 \times 40 = 1600$ pixels, with $H = 1600$ hidden dimensions and $H' = 34$

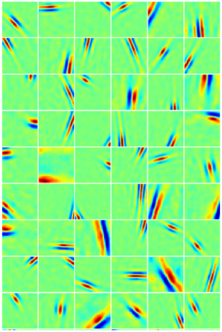


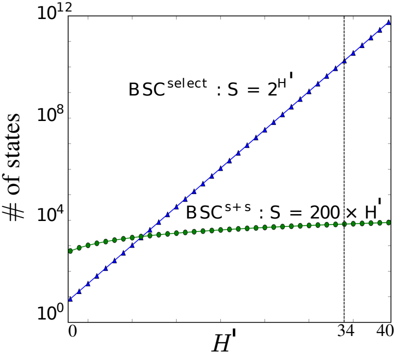
- Experiments: binary sparse coding for:
  (1) selection alone, (2) sampling alone, and
  (3) selection + sampling

Experiments – 3. Large scale on image patches

1600 latent dimensions with sampling-based posterior

W_h





- Shown: handful of the inferred basis functions W_h and comparison the of computational complexity for selection and select and sample

$\rightarrow$ Select and sample scales linearly with H'; selection exponentially

Summary

To **summer**-ize...

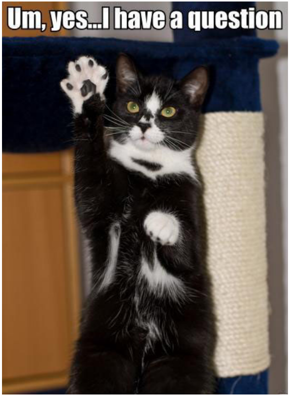
- Method scales well to high dimensional data (i.e. $H = 1600$)
- ...while maintaining sampling-based representation of posterior
- All model parameters learnable
- Combined approach represents reduced complexity and increased efficiency

Future/current:

- Generalized sparse coding
  - continuous hidden variables
  - compare diff inference methods (other variational, samplers)
- Generalized select-and-sample approach
  - try with other models

Thanks!

Thanks for your attention! Questions?



Appendix - References

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Appendix - Free-energy for latent variable models

Observed data $\mathcal{X} = \{\mathbf{x}_i\}$; Latent variables $\mathcal{Y} = \{\mathbf{y}_i\}$; Parameters θ.

Goal: Maximize the log likelihood (i.e. ML learning) wrt θ:

$$\ell(\theta) = \log P(\mathcal{X}|\theta) = \log \int P(\mathcal{Y}, \mathcal{X}|\theta) d\mathcal{Y},$$

Any distribution, $q(\mathcal{Y})$, over the hidden variables can be used to obtain a lower bound on the log likelihood using Jensen's inequality:

$$\ell(\theta) = \log \int q(\mathcal{Y}) \frac{P(\mathcal{Y}, \mathcal{X}|\theta)}{q(\mathcal{Y})} \, d\mathcal{Y} \geq \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}, \mathcal{X}|\theta)}{q(\mathcal{Y})} \, d\mathcal{Y} \stackrel{\text{def}}{=} \mathcal{F}(q, \theta).$$

Now,

$$\begin{aligned} \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}, \mathcal{X}|\theta)}{q(\mathcal{Y})} \, d\mathcal{Y} &= \int q(\mathcal{Y}) \log P(\mathcal{Y}, \mathcal{X}|\theta) \, d\mathcal{Y} - \int q(\mathcal{Y}) \log q(\mathcal{Y}) \, d\mathcal{Y} \\ &= \int q(\mathcal{Y}) \log P(\mathcal{Y}, \mathcal{X}|\theta) \, d\mathcal{Y} + \mathbf{H}[q], \end{aligned}$$

where $\mathbf{H}[q]$ is the entropy of $q(\mathcal{Y})$.
So:

$$\mathcal{F}(q, \theta) = \langle \log P(\mathcal{Y}, \mathcal{X}|\theta) \rangle_{q(\mathcal{Y})} + \mathbf{H}[q]$$

Appendix - Free-energy: E-step

The free energy can be re-written

$$\begin{aligned}
\mathcal{F}(q,\theta) &= \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y},\mathcal{X}|\theta)}{q(\mathcal{Y})}\, d\mathcal{Y} \\
&= \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}|\mathcal{X},\theta)P(\mathcal{X}|\theta)}{q(\mathcal{Y})}\, d\mathcal{Y} \\
&= \int q(\mathcal{Y}) \log P(\mathcal{X}|\theta)\, d\mathcal{Y} + \int q(\mathcal{Y}) \log \frac{P(\mathcal{Y}|\mathcal{X},\theta)}{q(\mathcal{Y})}\, d\mathcal{Y} \\
&= \ell(\theta) - \textbf{KL}[q(\mathcal{Y}) \| P(\mathcal{Y}|\mathcal{X},\theta)]
\end{aligned}$$

The second term is the Kullback-Leibler divergence.

This means that, for fixed θ, $\mathcal{F}$ is bounded above by ℓ, and achieves that bound when **KL**$[q(\mathcal{Y}) \| P(\mathcal{Y}|\mathcal{X},\theta)] = 0$.

But **KL**$[q \| p]$ is zero if and only if $q = p$. So, the E step simply sets

$$q^{(k)}(\mathcal{Y}) = P(\mathcal{Y}|\mathcal{X},\theta^{(k-1)})$$

and, after an E step, the free energy equals the likelihood.

Appendix - EM and neural processing

M-step equations for binary sparse coding:

$$W^{\rm new} = \left(\sum_{n=1}^{N} \vec{y}^{(n)} \, \langle \vec{s} \rangle_{q_n}^{T} \right) \left(\sum_{n=1}^{N} \left\langle \vec{s}\,\vec{s}^{\,T} \right\rangle_{q_n} \right)^{-1},$$

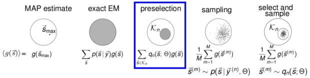
$$(\sigma^2)^{\rm new} = \frac{1}{ND} \sum_{n} \left\langle \left\| \vec{y}^{(n)} - W\,\vec{s} \right\|^2 \right\rangle_{q_n}$$

$$\pi^{\rm new} = \frac{1}{N} \sum_{n} \left| < \vec{s} >_{q_n} \right|, \text{ where } |\vec{x}| = \frac{1}{H} \sum_h x_h.$$

The EM iterations can be associated with neural processing by the

assumption that neural activity represents the posterior over hidden variables (E-step), and that synaptic plasticity implements changes to model parameters (M-step).

Appendix - Select and Sample



- **Selection**: Restrict approximate posterior to pre-selected states:

$$p(\vec{s}\,|\,\vec{y}^{\,(n)},\Theta) \approx q_n(\vec{s};\Theta) = \frac{p(\vec{s}\,|\,\vec{y}^{\,(n)},\Theta)}{\sum_{\vec{s}\,'\in\mathcal{K}_n} p(\vec{s}\,'\,|\,\vec{y}^{\,(n)},\Theta)}\,\delta(\vec{s}\in\mathcal{K}_n) \qquad (1)$$

- Choose set $\mathcal{K}_n$ w/ *selection function* $\mathcal{S}_h(\vec{y},\Theta)$; efficiently selects candidates s_h with most posterior mass:

$$\mathcal{K}_n = \{\vec{s}\,|\,\text{for all } h \notin \mathcal{I}_n : \; s_h = 0\}$$

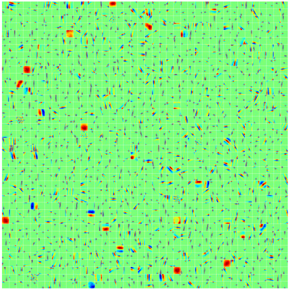
  where $\mathcal{I}_n$ contains the H' indices h with the highest values of $\mathcal{S}_h(\vec{y}^{\,(n)},\Theta)$, most likely contributors

- Can be seen as variational approximation to posterior
- Efficiently computable expectations in $\mathcal{O}(|\mathcal{K}_n|)$:

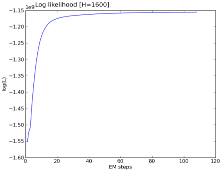
$$\langle g(\vec{s})\rangle_{p(\vec{s}\,|\,\vec{y}^{\,(n)},\Theta)} \approx \langle g(\vec{s})\rangle_{q_n(\vec{s};\Theta)} = \frac{\sum_{\vec{s}\in\mathcal{K}_n} p(\vec{s},\vec{y}^{\,(n)}\,|\,\Theta)\,g(\vec{s})}{\sum_{\vec{s}\,'\in\mathcal{K}_n} p(\vec{s}\,',\vec{y}^{\,(n)}\,|\,\Theta)} \qquad (2)$$

Appendix - Experimental results

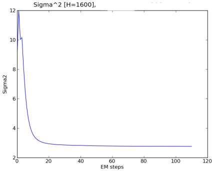
Select and sample on 40×40 image patches



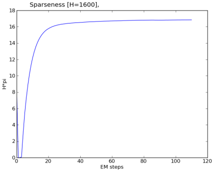
(a) Learned W bases.



(b) Log-likelihood

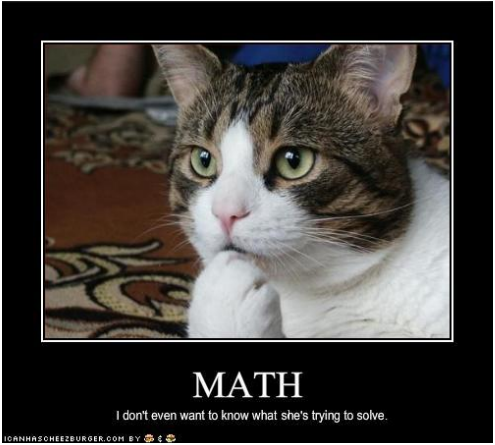


(c) Learned σ^2.



(d) Learned $\pi H'$.

Just a kitty


MATH
I don't even want to know what she's trying to solve.
ICANHASCHEEZBURGER.COM BY