Inference via Sampling (Contd)

Piyush Rai

Topics in Probabilistic Modeling and Inference (CS698X)

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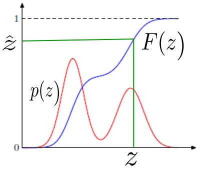
Recap: Basic Sampling Methods

- Inverse CDF method. Assume $F(z)$ to be CDF of our distribution of interest $p(z)$

$$\hat{z} \sim \text{Uniform}(0, 1)$$
$$z = F^{-1}(\hat{z})$$



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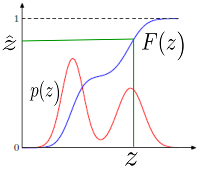

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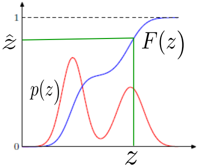

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- Note: The above are examples of the more general idea of transformation of distributions

$$p(\boldsymbol{z}) = q(\hat{\boldsymbol{z}}) \left| \frac{\partial \hat{\boldsymbol{z}}}{\partial \boldsymbol{z}} \right|$$

.. where $\left| \frac{\partial \hat{\boldsymbol{z}}}{\partial \boldsymbol{z}} \right|$ is the determinant of the Jacobian

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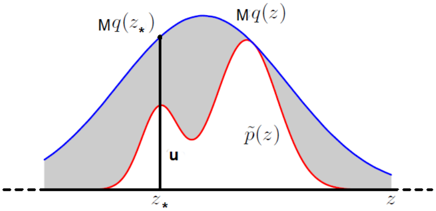

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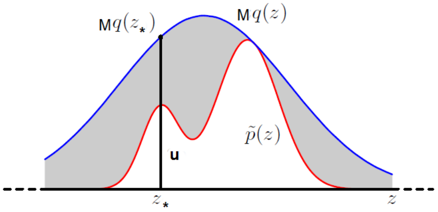

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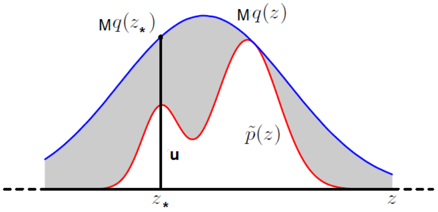

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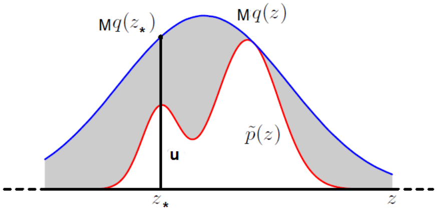

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  - Repeat the above two steps until we have generated the desired number of samples

Computing Expectations via Monte Carlo Sampling

- Often we are interested in computing expectations of the form

$$\mathbb{E}[f] = \int f(\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z}$$

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- Note that the variance in the estimate of expectation decreases as L increases

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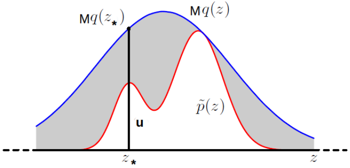

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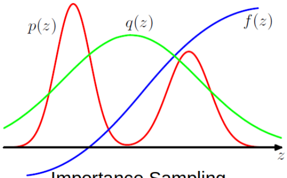

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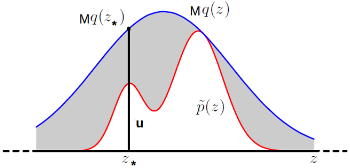

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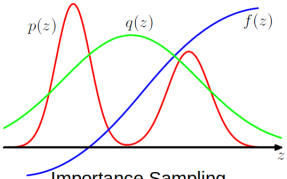

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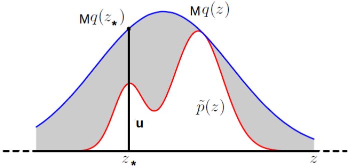

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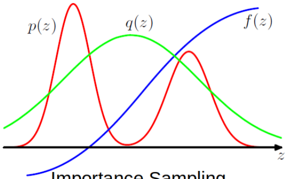

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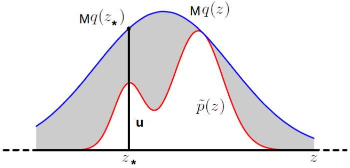

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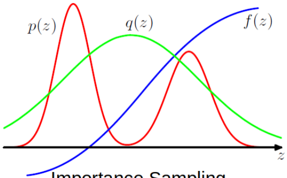

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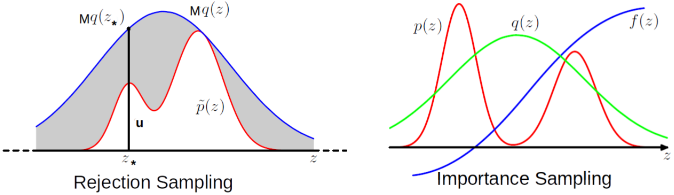

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  - Accept/reject $\boldsymbol{z}^*$ as the next sample based on an acceptance criterion (will see later)

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- Assume we can evaluate $p(\boldsymbol{z})$ at least up to a proportionality constant (i.e., can compute $\tilde{p}(\boldsymbol{z})$)
- Basic idea: MCMC uses a Markov Chain which, when converged, starts giving samples from $p(\boldsymbol{z})$

$$\underbrace{\boldsymbol{z}^{(1)} \rightarrow \boldsymbol{z}^{(2)} \rightarrow \boldsymbol{z}^{(3)} \rightarrow}_{\text{initial samples typically garbage}} \dots \rightarrow \underbrace{\boldsymbol{z}^{(L-2)} \rightarrow \boldsymbol{z}^{(L-1)} \rightarrow \boldsymbol{z}^{(L)}}_{\text{after convergence, actual samples from } p(\boldsymbol{z})}$$

- Given a current sample $\boldsymbol{z}^{(\ell)}$ from the chain, MCMC generates the next sample $\boldsymbol{z}^{(\ell+1)}$ as
  - Use a proposal distribution $q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$ to generate a candidate sample $\boldsymbol{z}^*$
  - Accept/reject $\boldsymbol{z}^*$ as the next sample based on an acceptance criterion (will see later)
  - If accepted, $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^*$. If rejected, $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^{(\ell)}$

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- Note that in MCMC, the proposal distribution $q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$ depends on the previous sample (unlike methods such as rejection sampling)

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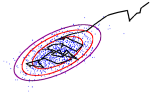
- MCMC chain run infinitely long (i.e., post-convergence) will give ONE sample from the target $p(\boldsymbol{z})$



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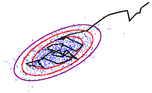

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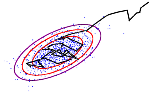

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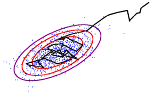

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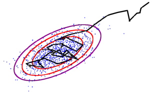

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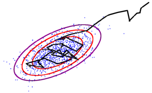

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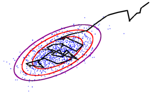

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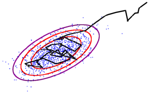

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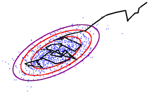

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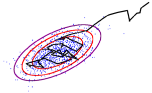

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  - Note: Good choices for T_1 and $T_i - T_{i-1}$ are usually based on heuristics
  - Note: MCMC is an approximate method because we don't usually know what T_1 is "long enough"

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- A first order Markov Chain assumes $p(\boldsymbol{z}^{(\ell+1)}|\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\ell)}) = p(\boldsymbol{z}^{(\ell+1)}|\boldsymbol{z}^{(\ell)})$

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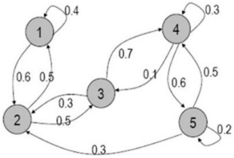
Transition probabilities can be defined using a *K*x*K* table if **z** is a discrete r.v. with *K* possible values

	1	2	3	4	5
1	0.4	0.6	0.0	0.0	0.0
2	0.5	0.0	0.5	0.0	0.0
3	0.0	0.3	0.0	0.7	0.0
4	0.0	0.0	0.1	0.3	0.6
5	0.0	0.3	0.0	0.5	0.2



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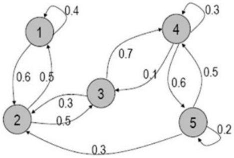

- Homogeneous Markov Chain: The TF is the same for all ℓ, i.e., $T_\ell = T$

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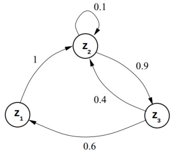

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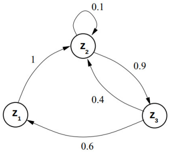

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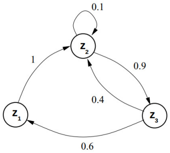

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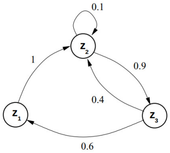

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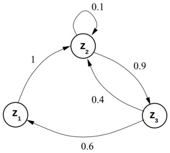

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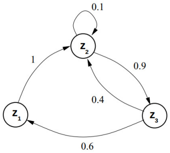

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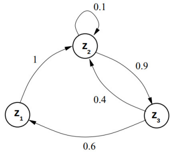

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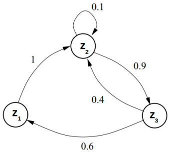

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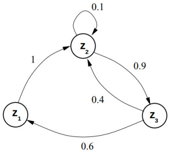
  - Irreducibility: T's graph is connected (ensures reachability from anywhere to anywhere)

MCMC: Some Basic Theory

- Consider the following simple TF with $K = 3$ (want to sample from a multinoulli)

$$T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix}$$



- Consider the initial state distribution $p(\boldsymbol{z}^{(0)}) = p(z_1^{(0)}, z_2^{(0)}, z_3^{(0)}) = [0.5, 0.2, 0.3]$
- Easy to see that $p(\boldsymbol{z}^{(0)}) \times T = [0.2, 0.6, 0.2] \Rightarrow$ distribution of $\boldsymbol{z}^{(1)}$
- Also easy to see that, after a few (say m) iterations, $p(\boldsymbol{z}^{(0)}) \times T^m = [0.2, 0.4, 0.4] = p(\boldsymbol{z})$ (say)
- For the above T, <u>any choice</u> of $p(\boldsymbol{z}^{(0)})$ leads to multinoulli $p(\boldsymbol{z})$i with $\pi = [0.2, 0.4, 0.4]$
  - Such a $p(\boldsymbol{z})$ is called the stationary/invariant distribution of this Markov Chain
- A Markov Chain has a stationary distribution if T has the following properties
  - Irreducibility: T's graph is connected (ensures reachability from anywhere to anywhere)
  - Aperiodicity: T's graph has no cycles (ensures that the chain isn't trapped in cycles)

MCMC: Some Basic Theory

- A sufficient (but not necessary) condition: A Markov Chain with transition function T has stationary distribution $p(\boldsymbol{z})$ if T satisfies Detailed Balance
- For any two states $\boldsymbol{z}$ and $\boldsymbol{z}'$, the Detailed Balanced condition is

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- Thus a Markov Chain with detailed balance will always converge to a stationary distribution

Some MCMC Algorithms

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- Exercise: Show that $T(\boldsymbol{z} \rightarrow \boldsymbol{z}^{(\tau)})$ satisfies the detailed balance property

$$T(\boldsymbol{z} \rightarrow \boldsymbol{z}^{(\tau)})p(\boldsymbol{z}) = T(\boldsymbol{z}^{(\tau)} \rightarrow \boldsymbol{z})p(\boldsymbol{z}^{(\tau)})$$

The MH Sampling Algorithm

- Initialize $\boldsymbol{z}^{(0)}$ randomly
- For $\ell = 0, \ldots, L-1$
  - Sample $\boldsymbol{z}^* \sim q(\boldsymbol{z}^*|\boldsymbol{z}^{(\ell)})$ and $u \sim \text{Unif}(0,1)$
  - If $u < A(\boldsymbol{z}^*, \boldsymbol{z}^{(\ell)}) = \min\left(1, \frac{\tilde{p}(\boldsymbol{z}^*)q(\boldsymbol{z}^{(\ell)}|\boldsymbol{z}^*)}{\tilde{p}(\boldsymbol{z}^{(\ell)})q(\boldsymbol{z}^*|\boldsymbol{z}^{(\ell)})}\right)$

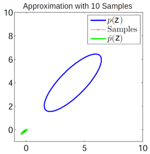
$$\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^* \qquad \text{(meaning: accepting with probability } A(\boldsymbol{z}^*, \boldsymbol{z}^{(\ell)}))$$

else

$$\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^{(\ell)}$$

MH Sampling in Action: A Toy Example..

Target $p(\boldsymbol{z}) = \mathcal{N}\left(\begin{bmatrix}4\\4\end{bmatrix}, \begin{bmatrix}1 & 0.8\\0.8 & 1\end{bmatrix}\right)$, Proposal $q(\boldsymbol{z}^{(t)}|\boldsymbol{z}^{(t-1)}) = \mathcal{N}\left(\boldsymbol{z}^{(t-1)}, \begin{bmatrix}0.01 & 0\\0 & 0.01\end{bmatrix}\right)$



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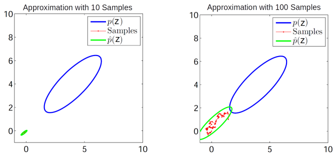

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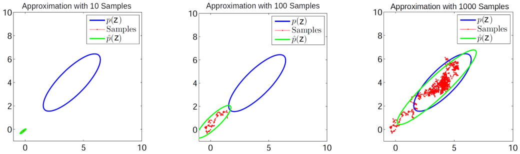

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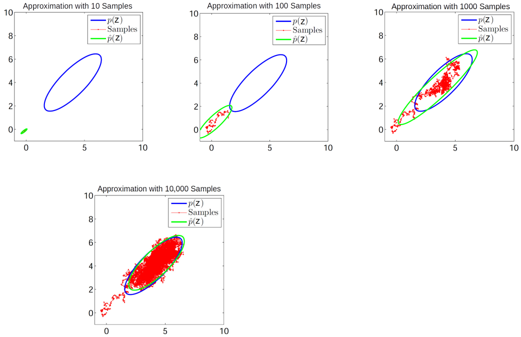

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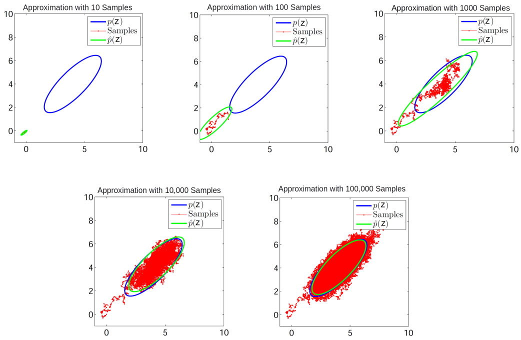

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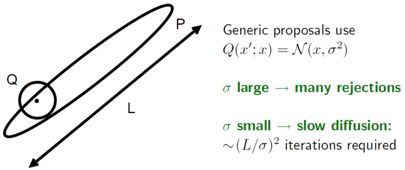

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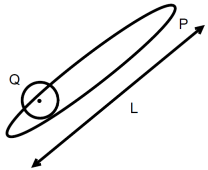

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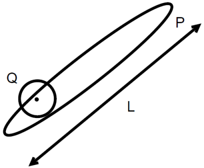

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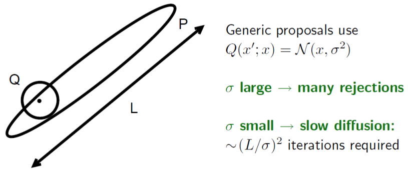

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$$A(\boldsymbol{z}^*, \boldsymbol{z}) = \frac{p(\boldsymbol{z}^*)q(\boldsymbol{z}|\boldsymbol{z}^*)}{p(\boldsymbol{z})q(\boldsymbol{z}^*|\boldsymbol{z})} = \frac{p(z_i^*|\boldsymbol{z}^*_{-i})p(\boldsymbol{z}^*_{-i})p(z_i|\boldsymbol{z}^*_{-i})}{p(z_i|\boldsymbol{z}_{-i})p(\boldsymbol{z}_{-i})p(z_i^*|\boldsymbol{z}_{-i})} = 1$$

where we use the fact that $\boldsymbol{z}^*_{-i} = \boldsymbol{z}_{-i}$

Gibbs Sampling: Sketch of the Algorithm

M: Total number of variables, T: number of Gibbs sampling steps

1. Initialize $\{z_i : i = 1, \ldots, M\}$
2. For $\tau = 1, \ldots, T$:
   - Sample $z_1^{(\tau+1)} \sim p(z_1 | z_2^{(\tau)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.
   - Sample $z_2^{(\tau+1)} \sim p(z_2 | z_1^{(\tau+1)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.

     $\vdots$
   - Sample $z_j^{(\tau+1)} \sim p(z_j | z_1^{(\tau+1)}, \ldots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \ldots, z_M^{(\tau)})$.

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Note: When sampling each variable from its conditional posterior, we use the most recent values of all other variables (this is akin to a co-ordinate ascent like procedure)

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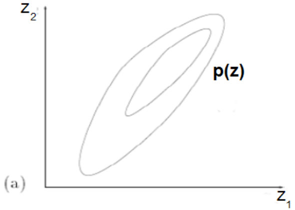
Note: Order of updating the variables *usually* doesn't matter (but see "Scan Order in Gibbs Sampling: Models in Which it Matters and Bounds on How Much" from NIPS 2016)

Gibbs Sampling: A Simple Example

Can sample from a 2-D Gaussian using 1-D Gaussians (recall that if the joint distribution is a 2-D Gaussian, conditionals will simply be 1-D Gaussians)



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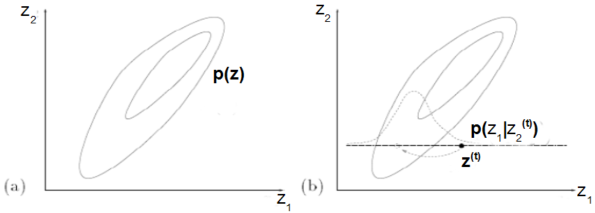

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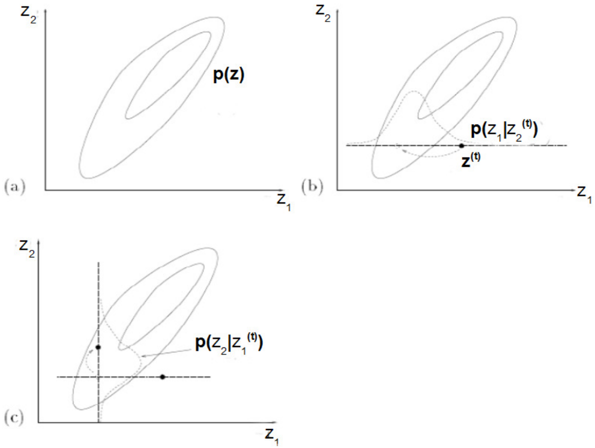

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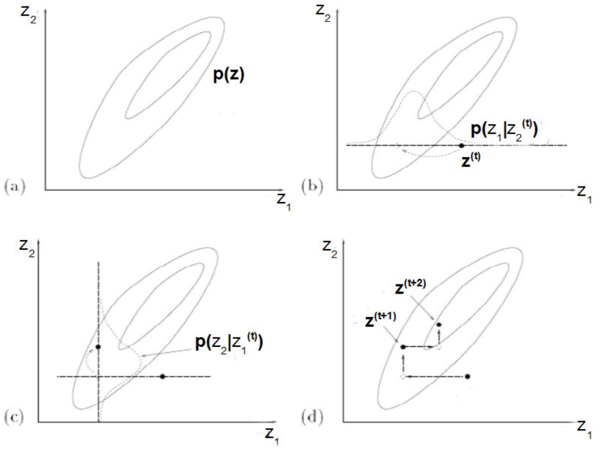

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  - Called the "Iterative Conditional Mode" (ICM) algorithm (doesn't give the posterior though)

Next Class

- Using posterior's gradient info in sampling algorithms
- Online MCMC algorithms
- Recent advances in MCMC
- Some other practical issues