

Notation	Explanation
$w_i$	Weight of $i$ th grid node
$\mathbf{W}$	$\{w_1, \dots, w_N\}$
$Z^{(k)} = \{i_1^{(k)}, \dots, i_{n^{(k)}}^{(k)}\}$	Path taken by trip $k$
$x_1^{(k)}, x_2^{(k)}$	Start and end locations of trip $k$
$\mathbf{Z}^{(k)} = \mathbf{Z}(x_1^{(k)}, x_2^{(k)})$	Set of reasonable paths for trip $k$
$T^{(k)}$	Time taken by trip $k$

Assume the following model

$$\begin{aligned}
\mathbf{W} &\sim p_{\mathbf{W}} \\
Z^{(k)} | \mathbf{W} &\sim p_{Z|\mathbf{W}} \quad (\text{a distribution over } \mathbf{Z}^{(k)}) \\
T^{(k)} | Z^{(k)}, \mathbf{W} &\sim \mathcal{N} \left( \sum_{i \in Z^{(k)}} w_i, \sigma^2 \right)
\end{aligned}$$

We are interested in the posterior distribution of  $\mathbf{W}$ :

$$\begin{aligned}
p(\mathbf{W} | T^{(k)}) &= \frac{p(T^{(k)} | \mathbf{W}) p(\mathbf{W})}{p(T^{(k)})} \\
&= \frac{[\sum_{Z^{(k)} \in \mathbf{Z}^{(k)}} p(T^{(k)} | Z^{(k)}, \mathbf{W}) p(Z^{(k)} | \mathbf{W})] p(\mathbf{W})}{p(T^{(k)})}
\end{aligned}$$

If we are only interested in the MAP, then we have

$$\log p(\mathbf{W} | T^{(k)}) = \underbrace{\log \left( \sum_{Z^{(k)} \in \mathbf{Z}^{(k)}} p(T^{(k)} | Z^{(k)}, \mathbf{W}) p(Z^{(k)} | \mathbf{W}) \right)}_{\ell(\mathbf{W} | T^{(k)}) \text{ log-likelihood}} + \underbrace{\log p(\mathbf{W})}_{\text{log prior}} + \text{const.}$$

Our main challenge here is to compute the log-likelihood, which involves a sum over all of  $\mathbf{Z}^{(k)}$ . If the set of reasonable paths include all paths inside a rectangle of size  $n \times m$ , then we have  $\binom{n+m}{n} \sim \frac{(n+m)^n}{n^n} e^n$  terms, which is clearly intractable. Zhan, et al. solves the issue by computing the 20 shortest path as the reasonable path set and then running softmax.

**Can we EM?** EM algorithm approximates the log-likelihood via

$$\begin{aligned}
Q(\mathbf{W} | \mathbf{W}^{(t)}) &= E [\log p(T^{(k)}, Z^{(k)} | \mathbf{W}) | T^{(k)}, \mathbf{W}^{(t)}] \\
&= -\frac{1}{2\sigma^2} \sum_{Z^{(k)} \in \mathbf{Z}^{(k)}} \left( T^{(k)} - \sum_{i \in Z^{(k)}} w_i \right)^2 p(Z^{(k)} | T^{(k)}, \mathbf{W}^{(t)}) + \text{const.}
\end{aligned}$$

However, (1) we again have to evaluate a sum of order  $|\mathbf{Z}|$  and (2) we don't have good estimates of  $p(Z^{(k)} | T^{(k)}, \mathbf{W}^{(t)})$ .

**Can we Monte Carlo?** We might consider using rejection sampling to approximate

$$E_Z [p(T^{(k)}|Z^{(k)}, \mathbf{W})|\mathbf{W}] \approx \frac{1}{L} \sum_{j=1}^L p(T^{(k)}|\tilde{Z}_j^{(k)}, \mathbf{W}).$$

The problem here is that the gradient update via `autograd` cannot take into account the gradient incurred *in the sampling process*.

**Can we variational inference?** Maybe. But (1) mean field doesn't really apply since  $Z^{(k)}$  cannot be broken into independent variables naturally and (2) VAE a la Kingma and Welling only works on continuous latent variables.

**A Monte Carlo based method** We repeatedly sample  $\tilde{Z}$  *uniformly* from  $\mathbf{Z}$  and use the sample mean to approximate summations over  $\mathbf{Z}$ .

$$\begin{aligned} & \log E_Z (p(T^{(k)}|Z^{(k)}, \mathbf{W})|\mathbf{W}) \\ &= \log \left[ |\mathbf{Z}| E_{\tilde{Z}} \left[ p(T^{(k)}|\tilde{Z}^{(k)}, \mathbf{W}) p(\tilde{Z}^{(k)}|\mathbf{W}) \right] \right] \quad (\text{where } \tilde{Z} \text{ is uniform over } \mathbf{Z}) \\ &= \log E_{\tilde{Z}} \left[ p(T^{(k)}|\tilde{Z}^{(k)}, \mathbf{W}) p(\tilde{Z}^{(k)}|\mathbf{W}) \right] + \text{const.} \\ &\geq E_{\tilde{Z}} \left[ \log p(T^{(k)}|\tilde{Z}^{(k)}, \mathbf{W}) \right] + E_{\tilde{Z}} \left[ \log p(\tilde{Z}^{(k)}|\mathbf{W}) \right] \quad (\text{Jensen; omitting constant}) \\ &= -\frac{1}{2L\sigma^2} \sum_{j=1}^L \left[ T^{(k)} - \sum_{i \in \tilde{Z}_j^{(k)}} w_i \right]^2 + \frac{1}{L} \sum_{i=1}^L \left[ -\sum_{i \in \tilde{Z}_j^{(k)}} w_i - \log \sum_{\mathbf{Z}} \exp \left( -\sum_{Z^{(k)}} w_i \right) \right] \\ &\quad (\text{We parameterize the distribution of } Z^{(k)} \text{ as Categorical with } \frac{\exp(-\sum w)}{\sum \exp(-\sum w)}) \\ &= -\frac{1}{2L\sigma^2} \sum_{j=1}^L \left[ T^{(k)} - \sum_{i \in \tilde{Z}_j^{(k)}} w_i \right]^2 - \frac{1}{L} \sum_{i=1}^L \sum_{i \in \tilde{Z}_j^{(k)}} w_i - \sum_{i=1}^L \log \left[ |\mathbf{Z}| E_{\tilde{Z}} \left[ \exp \left( -\sum_{\tilde{Z}} w_i \right) \right] \right] \\ &= -\frac{1}{2L\sigma^2} \sum_{j=1}^L \left[ T^{(k)} - \sum_{i \in \tilde{Z}_j^{(k)}} w_i \right]^2 - \frac{1}{L} \sum_{i=1}^L \sum_{i \in \tilde{Z}_j^{(k)}} w_i - \sum_{i=1}^L \log \text{sumexp}_{i=1, \dots, L} \left( -\sum_{\tilde{Z}_i} w_i \right) \end{aligned}$$