Probabilistic Machine Learning
Lecture 23
EM

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A special option: The EM algorithm

Maximizing model Evidence

<u>The general recipe</u> for hyperparameter inference:
Consider a model with **parameters $\boldsymbol{\theta}$**, **observed data $\boldsymbol{y}$** and **latent variables z**

- Ideally, we would like to maximize the **marginal (log-) likelihood (evidence)**

$$\log p(\boldsymbol{y} \mid \boldsymbol{\theta}) = \log \left(\int p(\boldsymbol{y}, z \mid \boldsymbol{\theta})\, dz \right) \qquad (\star)$$

- if we can not do this integral, we can try **Laplace**. This is nearly always *possible* (if $\log p(\boldsymbol{y} \mid z)$ is twice differentiable), but it is fundamentally an approximation.
- however, *in some cases*, we may be able to compute the Expectation **of the "complete data" log likelihood** (for a fixed value $\boldsymbol{\theta}_*$)

$$q(\boldsymbol{\theta}, \boldsymbol{\theta}_*) = \int p(z \mid \boldsymbol{y}, \boldsymbol{\theta}_*) \log p(\boldsymbol{y}, z \mid \boldsymbol{\theta})\, dz$$

and then Maximize $q(\boldsymbol{\theta}, \boldsymbol{\theta}_*)$ **with respect to $\boldsymbol{\theta}$**. This can be easier than $(\star)$ because the log "simplifies things" (e.g. turns products into sums, thus factors into components).

The EM Algorithm

Dempster, Laird, Rubin, *Maximum likelihood from incomplete data via the EM algorithm*, RSS B **39** (1) 1977, 1–38

Definition: The **Expectation Maximizatiion (EM)** algorithm:
Consider a model with **parameters** $\boldsymbol{\theta}$, **observed data** $\boldsymbol{y}$ and **latent variables** $\boldsymbol{z}$.

```
while not converged, do:
```

E compute the **Expected complete data log-likelihood**

$$q(\boldsymbol{\theta}, \boldsymbol{\theta}_t) = \int p(\boldsymbol{z} \mid \boldsymbol{y}, \boldsymbol{\theta}_t) \log p(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\theta}) \, d\boldsymbol{z}$$

M Set θ_{t+1} to **Maximize** $\boldsymbol{\theta}_{t+1} = \arg\max_{\boldsymbol{\theta}} q(\boldsymbol{\theta}, \boldsymbol{\theta}_{t+1})$.

EM is an attempt to maximize the evidence $p(\boldsymbol{y} \mid \boldsymbol{\theta})$. Why does it work?

An Observation

maximizing a lower bound

- We constructed an approximate distribution $q(z) = p(z \mid x, \theta)$ for our latent quantity
- For *any* such approximation $q(z)$ (if $q(z) > 0$ wherever $p(x, z \mid \theta) > 0$):

$$\begin{aligned} \log p(x \mid \theta) &= \log \int p(x, z \mid \theta)\, dz && = \log \int q(z) \frac{p(x, z \mid \theta)}{q(z)}\, dz \\ &\geq \int q(z) \log \frac{p(x, z \mid \theta)}{q(z)}\, dz && =: \mathcal{L}(q) \end{aligned}$$

Theorem (Jensen's (1906) inequality)

Let (Ω, A, μ) be a probability space, g be a real-valued, μ-integrable function and ϕ be a convex function on the real line. Then

$$\phi\left(\int_\Omega g\, d\mu\right) \leq \int_\Omega \phi \circ g\, d\mu.$$

An Observation

maximizing a lower bound

- We constructed an approximate distribution $q(z) = p(z \mid x, \theta)$ for our latent quantity
- For *any* such approximation $q(z)$ (if $q(z) > 0$ wherever $p(x, z \mid \theta) > 0$):

$$
\begin{aligned}
\log p(x \mid \theta) = \log \int p(x, z \mid \theta)\, dz \qquad & = \log \int q(z) \frac{p(x, z \mid \theta)}{q(z)}\, dz \\
\geq \int q(z) \log \frac{p(x, z \mid \theta)}{q(z)}\, dz \qquad & =: \mathcal{L}(q)
\end{aligned}
$$

- Thus, by maximizing the RHS in θ in the M-step, we increase a **lower bound on the Evidence**
- $\mathcal{L}(q)$ is thus called the **Evidence Lower Bound** (ELBO)
- But can we be sure that this increases the Evidence? To show that this is the case, we will now establish that the E-step makes the bound *tight* at the local θ.

An Insight

Distance of our bound

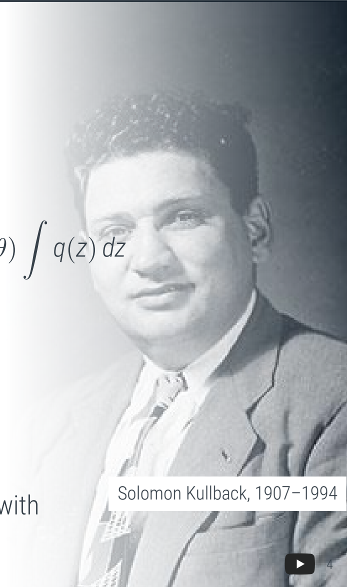
Richard A. Leibler, 1914–2003

$$
\begin{aligned}
\mathcal{L}(q) &= \int q(z) \log \frac{p(x, z \mid \theta)}{q(z)} \, dz \\
&= \int q(z) \log \frac{p(z \mid x, \theta) \cdot p(x \mid \theta)}{q(z)} \, dz \\
&= \int q(z) \log \frac{p(z \mid x, \theta)}{q(z)} \, dz + \log p(x \mid \theta) \int q(z) \, dz
\end{aligned}
$$

thus

$$
\begin{aligned}
\log p(x \mid \theta) &= \mathcal{L}(q) - \int q(z) \log \frac{p(z \mid x, \theta)}{q(z)} \\
&= \mathcal{L}(q) + D_{\mathrm{KL}}(q \| p(z \mid x, \theta))
\end{aligned}
$$

The Kullback-Leibler divergence satisfies $D_{\mathrm{KL}}(q\|p) \geq 0$ with $D_{\mathrm{KL}}(q\|p) = 0 \quad \Leftrightarrow q \equiv p$



Solomon Kullback, 1907–1994

EM maximizes the ELBO / minimizes Free Energy

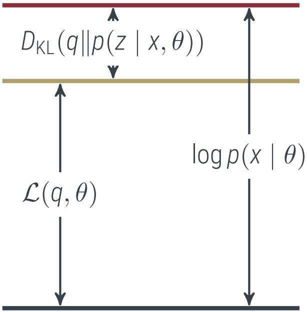
a more general view

exposition based on C.M. Bishop, 2006 §9.4

$$\log p(x \mid \theta) = \mathcal{L}(q, \theta) + D_{\mathrm{KL}}(q \| p(z \mid x, \theta))$$

$$\mathcal{L}(q, \theta) = \int q(z) \log \left(\frac{p(x, z \mid \theta)}{q(z)} \right) dz$$

$$D_{\mathrm{KL}}(q \| p(z \mid x, \theta)) = - \int q(z) \log \left(\frac{p(z \mid x, \theta)}{q(z)} \right) dz$$



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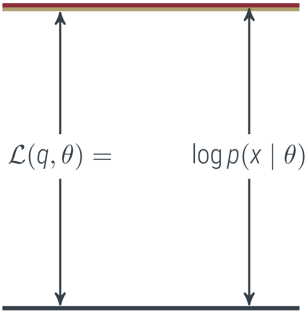
E -step: $q(z) = p(z \mid x, \theta_{\text{old}})$, thus $D_{\mathrm{KL}}(q \| p(z \mid x, \theta_i)) = 0$



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$$\log p(x \mid \theta) = \mathcal{L}(q,\theta) + D_{\mathrm{KL}}(q \| p(z \mid x,\theta))$$

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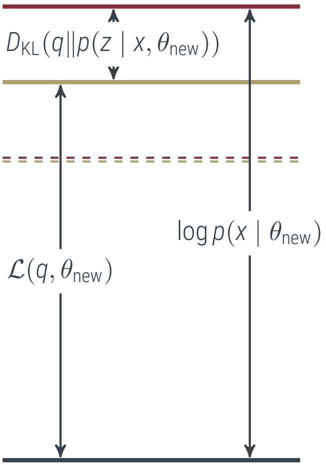
E -step: $q(z) = p(z \mid x, \theta_{\mathrm{old}})$, thus $D_{\mathrm{KL}}(q \| p(z \mid x, \theta_i)) = 0$

M -step: **Maximize ELBO**

$$\theta_{\mathrm{new}} = \arg\max_\theta \int q(z) \log p(x,z \mid \theta)\, dz$$

$$= \arg\max_\theta \mathcal{L}(q,\theta) + \int q(z) \log q(z)\, dz$$



EM Algorithm — General Form

summary

exposition based on C.M. Bishop, 2006 §9.4

Setting: Want to find *maximum likelihood* (or MAP) estimate for a model involving a **latent** variable

$$\theta_* = \arg\max_\theta \left[\log p(x \mid \theta)\right] = \arg\max_\theta \left[\log\left(\int p(x, z \mid \theta)\, dz\right)\right]$$

Algorithm: Initialize θ_0, then iterate:

1. Compute $q(z) = p(z \mid x, \theta_{\text{old}})$, thereby setting $D_{\text{KL}}(q \| p(z \mid x, \theta)) = 0$
2. Set θ_{new} to the **Maximize** the **Evidence Lower Bound**

$$\theta_{\text{new}} = \arg\max_\theta \mathcal{L}(q, \theta) = \arg\max_\theta \int q(z) \log\left(\frac{p(x, z \mid \theta)}{q(z)}\right) dz$$

3. Check for convergence of either the log likelihood, or θ.

EM for MAP

dealing with the data is the main challenge, adding a prior is easy

- It is straightforward to extend EM to maximize a **posterior** instead of a likelihood. Just add a log prior for θ:

Initialize θ_0, then iterate between

1. Compute $q(z) = p(z \mid x, \theta_{\text{old}})$, thereby setting $D_{\text{KL}}(q \| p(z \mid x, \theta)) = 0$
2. Set θ_{new} to the **Maximize** the **Evidence Lower Bound**

$$\theta_{\text{new}} = \arg\max_{\theta} \int q(z) \log \left(\frac{p(x, z \mid \theta) p(\theta)}{q(z)} \right) dz = \arg\max_{\theta} \mathcal{L}(q, \theta) + \log p(\theta)$$

3. Check for convergence of either the log likelihood, or θ.

This maximizes

$$\begin{aligned} \log p(x \mid \theta) + \log p(\theta) &\geq \mathcal{L}(q, \theta) + \log p(\theta) \\ &\triangleq \log p(\theta \mid x) \end{aligned}$$

Another Observation

why is it even useful to build an iterative update in this way?

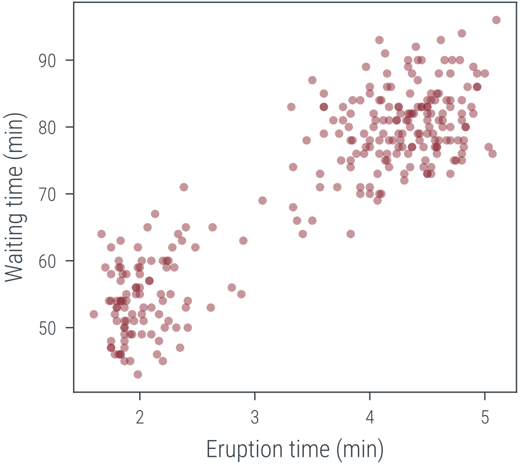
If $p(x, z \mid \theta)$ is an **exponential family** with θ as the natural parameters, then

$$
\begin{aligned}
p(x,z) &= \exp(\phi(x,z)^\intercal\theta - \log Z(\theta)) \\
\mathcal{L}(q(z),\theta) &= \mathbb{E}_{q(z)}(\phi(x,z)^\intercal\theta - \log Z(\theta)) = \mathbb{E}_{q(z)}[\phi(x,z)]^\intercal\theta - \log Z(\theta) \\
\nabla_\theta\mathcal{L}(q(z),\theta) = 0 \quad &\Rightarrow \quad \nabla_\theta \log Z(\theta) = \mathbb{E}_{p(x,z)}[\phi(x,z)] = \mathbb{E}_{q(z)}[\phi(x,z)]
\end{aligned}
$$

and optimization may be analytic (example below: Gaussian Mixture Models).

Example

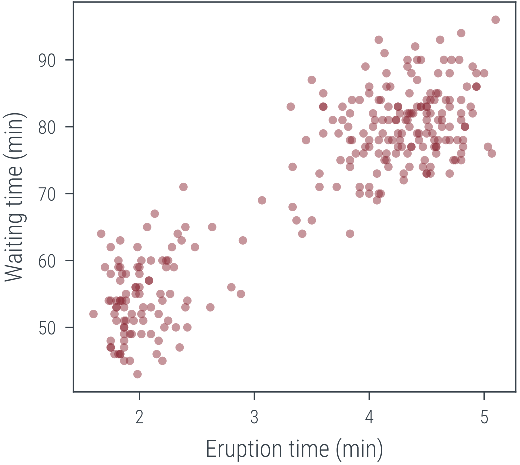
Gaussian Mixture Models



$$p(\boldsymbol{x} \mid \pi, \mu, \Sigma) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_n \mid \mu_k, \Sigma_k),$$

$$\pi_k \in [0, 1], \sum_k \pi_k = 1$$

$$p(\boldsymbol{x}, \boldsymbol{z} \mid \pi, \mu, \Sigma) = \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(x_n \mid \mu_k, \Sigma_k)^{z_{nk}}$$

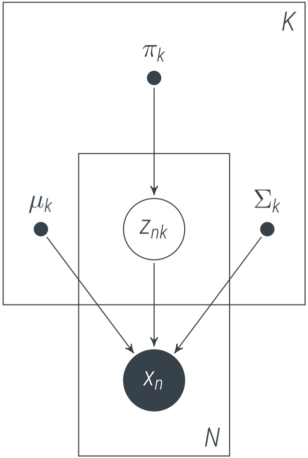


EM for Gaussian Mixtures

introducing a class membership variable z factorizes the likelihood

- Want to maximize, as function of $\theta := (\pi_k, \mu_k, \Sigma_k)_{k=1,\dots,K}$

$$\log p(x \mid \pi, \mu, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k) \right)$$



EM for Gaussian Mixtures

introducing a class membership variable z factorizes the likelihood

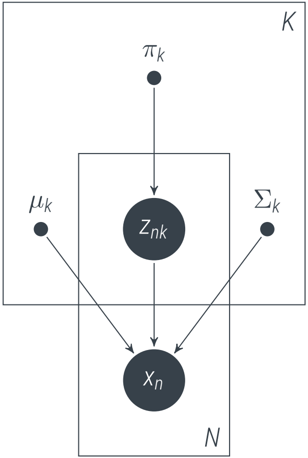
- Want to maximize, as function of $\theta := (\pi_k, \mu_k, \Sigma_k)_{k=1,\dots,K}$

$$\log p(x \mid \pi, \mu, \Sigma) = \sum_{n=1}^{N} \log \left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k) \right)$$

- Instead, maximizing the "complete data" likelihood is easier:

$$\log p(x, z \mid \pi, \mu, \Sigma) = \log \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(x_n; \mu_k, \Sigma_k)^{z_{nk}}$$

$$= \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \underbrace{(\log \pi_k + \log \mathcal{N}(x_n; \mu_k, \Sigma_k))}_{\text{easy to optimize (exponential families!)}}$$



E-Step: Compute $p(z \mid x, \theta)$:

$$p(z_{nk} = 1 \mid x_n, \pi, \mu, \Sigma) = \frac{p(z_{nk} = 1) p(x_n \mid z_{nk} = 1)}{\sum_{k'=1}^K p(z_{nk'} = 1) p(x_n \mid z_{nk'} = 1)}$$

$$= \frac{\pi_k \mathcal{N}(x_n; \mu_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(x_n; \mu_{k'}, \Sigma_{k'})} =: r_{nk}$$

Note that discrete distributions $q(z_{nk} = 1) = r_{nk}$ have expectation $\mathbb{E}_q[z_{nk}] = r_{nk}$

M-Step: Maximize ELBO

$$\mathbb{E}_{p(\mathbf{z}|\mathbf{x},\theta)} \left(\log p(\mathbf{x}, \mathbf{z} \mid \theta) \right) = \sum_{n=1}^N \sum_{k=1}^K r_{nk} \left(\log \pi_k + \log \mathcal{N}(x_n; \mu_k, \Sigma_k) \right)$$

EM for Gaussian Mixtures

M-step derivations

$$\mathbb{E}_{p(\boldsymbol{z}|\boldsymbol{x},\theta)}\left(\log p(\boldsymbol{x},\boldsymbol{z}\mid\theta)\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\left(\log \pi_k + \log \mathcal{N}(x_n;\mu_k,\Sigma_k)\right)$$

To maximize w.r.t. μ set gradient of ELBO to 0:

$$\nabla_{\mu_\ell}\mathbb{E}_{p(\boldsymbol{z}|\boldsymbol{x},\theta)}\left(\log p(\boldsymbol{x},\boldsymbol{z}\mid\theta)\right) = -\sum_{n=1}^{N} r_{n\ell}\Sigma_\ell^{-1}(x_n-\mu_\ell) \overset{!}{=} 0$$

$$\Rightarrow \quad \mu_\ell = \frac{1}{R_\ell}\sum_{n=1}^{N} r_{n\ell}x_n \qquad R_j := \sum_{n=1}^{N} r_{n\ell}$$

EM for Gaussian Mixtures

M-step derivations

$$\mathbb{E}_{p(\mathbf{z}|\mathbf{x},\theta)}\left(\log p(\mathbf{x},\mathbf{z} \mid \theta)\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\left(\log \pi_k + \log \mathcal{N}(x_n;\mu_k,\Sigma_k)\right)$$

To maximize w.r.t. Σ set gradient of ELBO to 0
(note $\partial|\Sigma|^{-1/2}/\partial\Sigma = -\frac{1}{2}|\Sigma|^{-3/2}|\Sigma|\Sigma^{-1}$ and $\partial(v^\intercal\Sigma^{-1}v)/\partial\Sigma = -\Sigma^{-1}vv^\intercal\Sigma^{-1}$):

$$\nabla_{\Sigma_\ell}\mathbb{E}_{p(\mathbf{z}|\mathbf{x},\theta)}\left(\log p(\mathbf{x},\mathbf{z} \mid \theta)\right) = -\frac{1}{2}\sum_{n=1}^{N} r_{n\ell}\left(\Sigma_\ell^{-1}(x_n-\mu_\ell)(x_n-\mu_\ell)^\intercal\Sigma_\ell^{-1} - \Sigma_\ell^{-1}\right)$$

$$\Rightarrow \quad \Sigma_\ell = \frac{1}{R_\ell}\sum_{n=1}^{N} r_{n\ell}(x_n-\mu_\ell)(x_n-\mu_\ell)^\intercal \qquad R_\ell := \sum_{n=1}^{N} r_{n\ell}$$

EM for Gaussian Mixtures

M-step derivations

$$\mathbb{E}_{p(\boldsymbol{z}|\boldsymbol{x},\theta)}\left(\log p(\boldsymbol{x},\boldsymbol{z}\mid\theta)\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\left(\log \pi_k + \log \mathcal{N}(x_n;\mu_k,\Sigma_k)\right)$$

To maximize w.r.t. π, enforce $\sum_k \pi_k = 1$ by introducing Lagrange multiplier λ and optimize

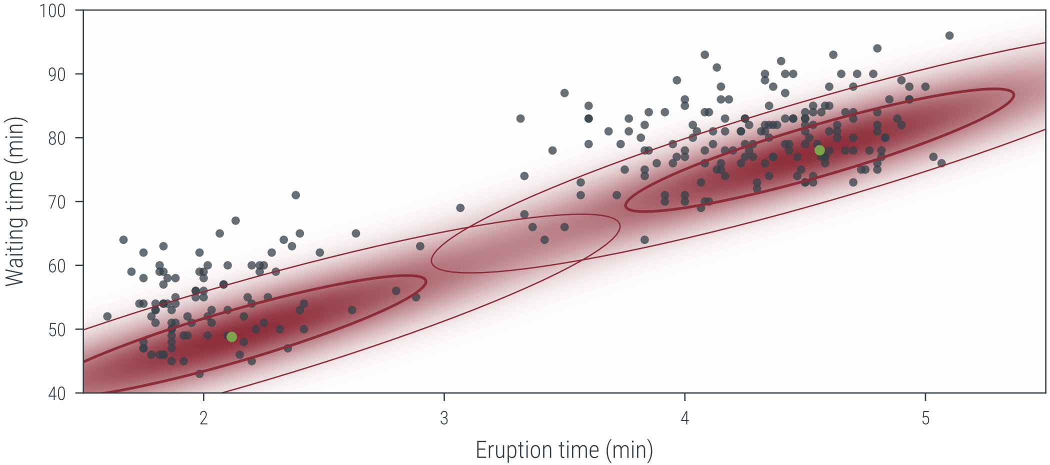
$$\nabla_{\pi_\ell}\mathbb{E}_{p(\boldsymbol{z}|\boldsymbol{x},\theta)}\left(\log p(\boldsymbol{x},\boldsymbol{z}\mid\theta)\right) + \lambda\left(\sum_{k=1}^{K}\pi_k - 1\right) = \sum_{n=1}^{N} r_{n\ell}\frac{1}{\pi_\ell} + \lambda \overset{!}{=} 0$$

$$\pi_\ell = -\frac{1}{\lambda}\sum_{n=1}^{N} r_{n\ell} = -\frac{1}{\lambda}R_\ell$$

$$\sum_{k=1}^{K}\pi_k = 1 \Rightarrow \lambda = -N \qquad \text{and} \qquad \pi_\ell = \frac{R_\ell}{N}$$

EM for Gaussian Mixtures

example run



EM for Gaussian Mixtures

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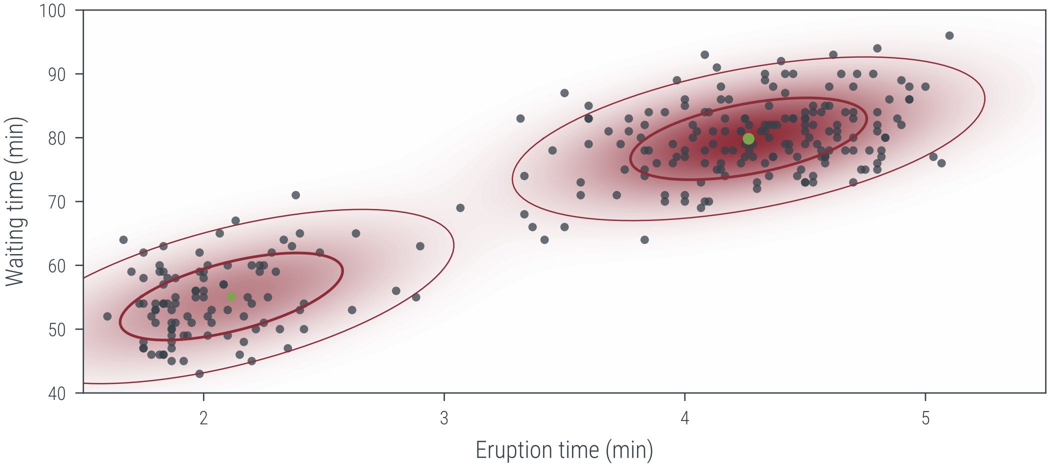

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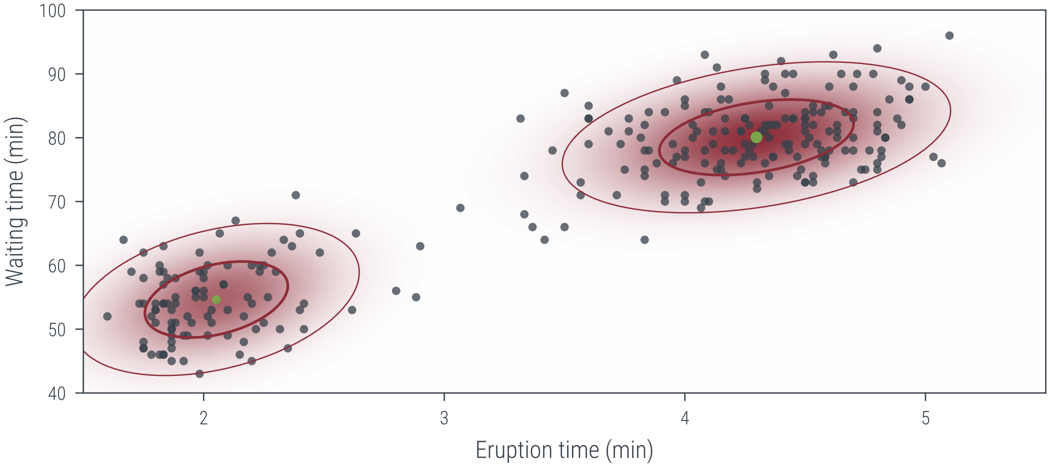

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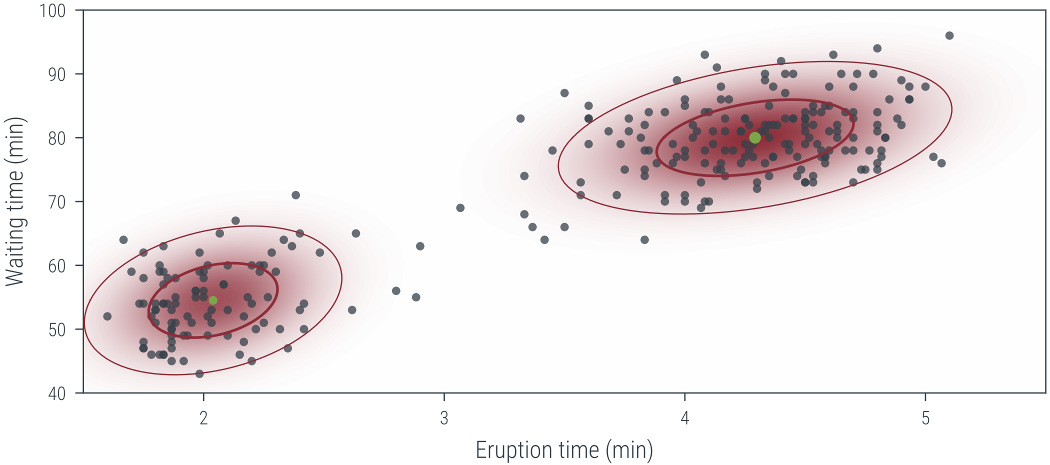

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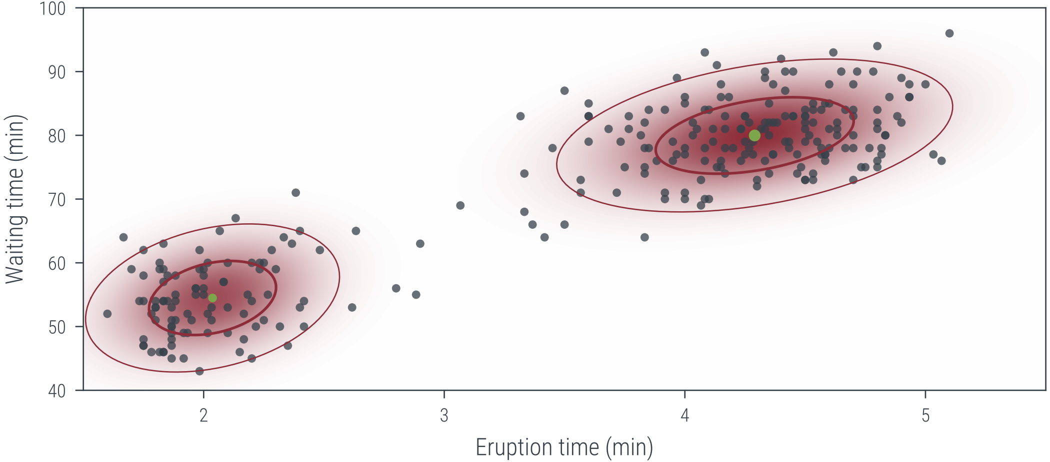

The EM algorithm:

- to find *maximum likelihood* (or MAP) estimate for a model involving a **latent** variable

$$\boldsymbol{\theta}_* = \arg\max_{\boldsymbol{\theta}} [\log p(\boldsymbol{x} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})] = \arg\max_{\boldsymbol{\theta}} \left[\log \left(\sum_{z} p(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) \right) \right]$$

- Initialize $\boldsymbol{\theta}_0$, then iterate (checking convergence of either the log likelihood, or $\boldsymbol{\theta}$)

E Compute $p(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{\theta}_{\text{old}})$, thereby setting $D_{\text{KL}}(q \| p(\boldsymbol{z} \mid \boldsymbol{x}, \boldsymbol{\theta}) = 0$

M Set $\boldsymbol{\theta}_{\text{new}}$ to the **Maximize** the **Expectation Lower Bound**

$$\boldsymbol{\theta}_{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{L}(q, \boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{z} q(\boldsymbol{z}) \log \left(\frac{p(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})}{q(\boldsymbol{z})} \right)$$

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