Note: Marginal likelihood for Bayesian models with a Gaussian-approximated posterior

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I first learned this solution from Botond Cseke. I'm not sure where it originates; It is a corollary of Laplace's method for approximating integrals using a Gaussian distribution.

If I have a Bayesian statistical model with hyperparameters Θ , with a no closed-form posterior, how can I optimize Θ ?

Consider a Bayesian statistical model with observed data $y \in \mathcal{Y}$ and hidden (latent) variables $z \in \mathcal{Z}$, which we infer. We have a prior on z, $Pr(z; \Theta)$, and a model for the probability of y given z (likelihood), $Pr(y|z; \Theta)$. The prior and likelihood are controlled by "hyperparameters" Θ , which we would like to estimate. Recall that Bayes theorem states:

$$Pr(\mathbf{z}|\mathbf{y};\Theta) = Pr(\mathbf{y}|\mathbf{z};\Theta) \frac{Pr(\mathbf{z};\Theta)}{Pr(\mathbf{y};\Theta)}$$
(1)

It is common for the posterior $Pr(\mathbf{z}|\mathbf{y}; \Theta)$ to lack a closed-form solution. In this case, one typically approximates the posterior with a more tractable distribution $Q(\mathbf{z}) \approx Pr(\mathbf{z}|\mathbf{y}; \Theta)$. Common ways of estimating (\mathbf{z}) include the Laplace approximation, variational Bayes, expectation propagation, and expectation maximization algorithms. The only approximating distribution in common use for high-dimensional \mathbf{z} is the multivariate Gaussian (or some nonlinear transformation thereof), which succinctly captures joint statistics with limited computational overhead. Assume we have an inference procedure which returns the approximate posterior $Q(\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_{q}, \boldsymbol{\Sigma}_{q})$.

We optimize the hyperparameters " Θ " of the prior kernel to maximize the marginal likelihood of the observations **y**

$$\theta \leftarrow \underset{\Theta}{\operatorname{argmax}} \Pr(\mathbf{y}; \Theta)$$
$$\Pr(\mathbf{y}; \Theta) = \int_{\mathcal{Z}} \Pr(\mathbf{y}, \mathbf{z}; \Theta) \, d\mathbf{z} = \int_{\mathcal{Z}} \Pr(\mathbf{y} | \mathbf{z}) \Pr(\mathbf{z}; \Theta) \, d\mathbf{z}$$
(2)

Except in rare special cases, this integral does not have a closed form. However, we have already obtained a Gaussian approximation to the posterior distribution, $Q(z) \approx \Pr(z|y;\Theta)$. If we replace $\Pr(z|y;\Theta)$ with our approximation Q(z) in this equation, we can solve for (an approximation) of $\Pr(y;\Theta)$:

$$Q(\mathbf{z}) \approx \Pr(\mathbf{y}|\mathbf{z}) \frac{\Pr(\mathbf{z};\Theta)}{\Pr(\mathbf{y};\Theta)} \Longrightarrow \Pr(\mathbf{y};\Theta) \approx \Pr(\mathbf{y}|\mathbf{z}) \frac{\Pr(\mathbf{z};\Theta)}{Q(\mathbf{z})}$$
(3)

Working in log-probability, and evaluating the expression at the (approximated) posterior mean $z = \mu_q$, we get

$$\ln \Pr(\mathbf{z}=\boldsymbol{\mu}_{q};\Theta) = -\frac{1}{2} \left\{ \ln |2\pi\boldsymbol{\Sigma}_{z}| + (\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{z})^{\top}\boldsymbol{\Sigma}_{z}^{-1}(\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{z}) \right\}$$

$$\ln Q(\mathbf{z}=\boldsymbol{\mu}_{q}) = -\frac{1}{2} \left\{ \ln |2\pi\boldsymbol{\Sigma}_{q}| + (\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{q})^{\top}\boldsymbol{\Sigma}_{q}^{-1}(\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{q}) \right\} = -\frac{1}{2} \ln |2\pi\boldsymbol{\Sigma}_{q}|$$

$$\ln \Pr(\mathbf{y};\Theta) \approx \ln \Pr(\mathbf{y}|\mathbf{z}=\boldsymbol{\mu}_{q};\Theta) + \ln \Pr(\mathbf{z}=\boldsymbol{\mu}_{q};\Theta) - \ln Q(\mathbf{z}=\boldsymbol{\mu}_{q})$$

$$= \ln \Pr(\mathbf{y}|\mathbf{z}=\boldsymbol{\mu}_{q};\Theta) - \frac{1}{2} \left\{ \ln |\boldsymbol{\Sigma}_{q}^{-1}\boldsymbol{\Sigma}_{z}| + (\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{z})^{\top}\boldsymbol{\Sigma}_{z}^{-1}(\boldsymbol{\mu}_{q}-\boldsymbol{\mu}_{z}) \right\}$$

$$(4)$$

This is quite tractable to compute.

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