

Kullback–Leibler divergence between multivariate Gaussians

The Kullback–Leibler divergence from distribution $p(x)$ to $q(x)$ is:

$$\text{KL}(p, q) = \mathbb{E}_p\{\log(p) - \log(q)\} = \int \log\left(\frac{p(x)}{q(x)}\right)p(x) dx$$

If $p = \mathcal{N}(\mu, \Sigma)$ and $q = \mathcal{N}(\nu, \Lambda)$ are **multivariate Gaussian distributions**, then

$$\log p = -\frac{D}{2} \log \tau - \frac{1}{2} \log |\Sigma| - \frac{1}{2} (x - \mu)^T \Sigma (x - \mu)$$

$$\log q = -\frac{D}{2} \log \tau - \frac{1}{2} \log |\Lambda| - \frac{1}{2} (x - \nu)^T \Lambda (x - \nu)$$

and so

$$\text{KL}(p, q) = \frac{1}{2} \log \frac{|\Sigma|}{|\Lambda|} - \frac{1}{2} \mathbb{E}_p\{(x - \mu)^T \Sigma^{-1} (x - \mu)\} + \frac{1}{2} \mathbb{E}_q\{(x - \nu)^T \Lambda^{-1} (x - \nu)\}$$

Since the terms are scalars, they are equal to their trace, allowing us to take the covariance matrices out of the expectation value:

$$\text{KL}(p, q) = \frac{1}{2} \log \frac{|\Sigma|}{|\Lambda|} - \frac{1}{2} \text{tr}[\mathbb{E}_p\{(x - \mu)(x - \mu)^T\} \Sigma^{-1}] + \frac{1}{2} \text{tr}[\mathbb{E}_q\{(x - \nu)(x - \nu)^T\} \Lambda^{-1}]$$

In more detail each term is rewritten as follows:

$$\begin{aligned} & \text{tr}[\mathbb{E}_p\{(x - \mu)^T \Sigma^{-1} (x - \mu)\}] \\ &= \mathbb{E}_p\{\text{tr}[(x - \mu)^T \Sigma^{-1} (x - \mu)]\} \\ &= \mathbb{E}_p\{\text{tr}[(x - \mu)(x - \mu)^T \Sigma^{-1}]\} \\ &= \text{tr}[\mathbb{E}_p\{(x - \mu)(x - \mu)^T \Sigma^{-1}\}] \\ &= \text{tr}[\mathbb{E}_p\{(x - \mu)(x - \mu)^T\} \Sigma^{-1}] \end{aligned}$$

Since $\mathbb{E}_p\{(x - \mu)(x - \mu)^T\} = \Sigma$ by definition, the first term becomes $\text{tr}[\Sigma \Sigma^{-1}] = D$, while the second can be rewritten as

$$\begin{aligned} & \mathbb{E}_p\{(x - \nu)(x - \nu)^T\} \\ &= \mathbb{E}_p\{((x - \mu) - (\nu - \mu))((x - \mu) - (\nu - \mu))^T\} \\ &= \mathbb{E}_p\{(x - \mu)(x - \mu)^T\} - (x - \mu)(\nu - \mu) - (\nu - \mu)(x - \mu) + (\nu - \mu)(\nu - \mu)^T \\ &= \Sigma + (\mu - \nu)(\mu - \nu)^T \end{aligned}$$

Pulling this together,

$$\begin{aligned} \text{KL}(p, q) &= \frac{1}{2} \log \frac{|\Lambda|}{|\Sigma|} - \frac{D}{2} + \frac{1}{2} \text{tr}[(\Sigma + (\mu - \nu)(\mu - \nu)^T) \Lambda^{-1}] \\ &= \frac{1}{2} \log \frac{|\Lambda|}{|\Sigma|} - \frac{D}{2} + \frac{1}{2} \text{tr}[\Sigma \Lambda^{-1}] + \text{tr}[(\mu - \nu)^T \Lambda^{-1} (\mu - \nu)] \end{aligned}$$

Univariate case

For $D = 1$, this result becomes:

$$\text{KL}(\mathcal{N}(\mu, \sigma^2), \mathcal{N}(\nu, \rho^2)) = \log \frac{\rho}{\sigma} + \frac{\sigma^2 + (\mu - \nu)^2}{2\rho^2} - \frac{1}{2}$$