Hybrid Monte Carlo: Test Distributions

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1) Mirrored Gaussians

The test distribution used in `main.cpp` is a mirrored multidimensional Gaussian distribution:

$$p(\vec{x}) = a\,\mathcal{N}(\vec{x};\vec{\mu},\Sigma) + b\,\mathcal{N}(\vec{x};-\vec{\mu},\Sigma) \ \ , \text{ where } a+b=1 \ . \tag{1}$$

where $\pm\,\vec{\mu}$ and Σ are the means and the covariance of of each Gaussian. This distribution is therefore composed of two wells of different depths symmetrically placed about the origin. The covariance of each Gaussian is the same, and is given by

$$\Sigma = \mathrm{diag}\big(\sigma_1^2,\, \ldots, \sigma_N^2\big) \ \ . \tag{2}$$

The mean μ' of the full distribution is given by

$$\vec{\mu}' = \int \mathrm{d}x\, x\, p(x) = (a-b)\,\vec{\mu} \ \ . \tag{3}$$

The second moment along each axis can be expressed in terms of μ_i and σ_i as follows:

$$\begin{aligned} \left\langle (x_i')^2 \right\rangle = \int \mathrm{d}x\, x^2\, p(x) &= a\left\langle x_{i,+}^2 \right\rangle + b\left\langle x_{i,-}^2 \right\rangle && (4) \\ &= (a+b)\left(\sigma_i^2 + \mu_i^2\right) && (5) \\ &= \sigma_i^2 + \mu_i^2 \ . && (6) \end{aligned}$$

The variance along a single axis is now easily obtained:

$$\begin{aligned} (\sigma_i')^2 &= (a+b)\left(\sigma_i^2 + \mu_i^2\right) - (a-b)^2\,\mu_i^2 && (7) \\ &= (a+b)\,\sigma_i^2 + \left[a+b-(a-b)^2\right]\mu_i^2 && (8) \\ &= \sigma_i^2 + \left[1-(a-b)^2\right]\mu_i^2 \ . && (9) \end{aligned}$$

This can in fact be extended to the full covariance matrix by substituting $\sigma_i^2 \to \Sigma_{ij}$ and $\mu_i^2 \to \langle x_i x_j \rangle$. For the off-diagonal terms, this simplifies to

$$\begin{aligned} \Sigma_{ij}' &= \Sigma_{ij} + \left[1-(a-b)^2\right]\langle x_i x_j \rangle && (10) \\ &= \left[1-(a-b)^2\right]\mu_i\,\mu_j \ . && (11) \end{aligned}$$