Here Be Hyper-Dragons: High-Dimensional Spaces and Statistical Computation

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TROGDOR the BURNINATOR
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If relevant neighborhoods are determined by *probability density* then we should focus computation near the mode.
But integration doesn’t just evaluate the integrand -- it aggregates it over volumes.

\[ E[f] = \int \pi(\theta) f(\theta) \]
Volume, however, starts to behave strangely as the dimension of our parameter space increases.
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The dominant contributions to an integral is dictated not by probability *density* but rather by probability *mass*.
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As the dimensionality increases, probability mass concentrates near a hypersurface called the *typical set*. 

\[ \pi(\theta) \, d\theta \]

\[ |\theta - \theta_{\text{Model}}| \]
This concentration of measure into a nearly singular typical set frustrates the accurate estimation of integrals.
In order to accurately approximating expectations computational methods must quantify the typical set.

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Variational methods optimize over a family of convenient approximating distributions.

\[ \pi(\theta) \]
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\[
\{q(\theta, \alpha)\}
\]
Variational methods optimize over a family of convenient approximating distributions.
The (local) variational solution is then used to approximate the target expectations.

\[ \pi(\theta) \approx q(\theta, \hat{\alpha}) \]

\[ \int f(\theta) \pi(\theta) \, d\theta \approx \int f(\theta) q(\theta, \hat{\alpha}) \, d\theta \]
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$$\pi(\theta)$$
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Stochastic methods construct estimators that converge to the exact target expectations.

$$\int f(\theta) \pi(\theta) \, d\theta \approx \frac{\sum_{n=1}^{N} w(\theta_n) f(\theta_n)}{\sum_{n=1}^{N} w(\theta_n)}$$
Monte Carlo methods quantify the typical set using exact samples drawn from the target distribution.
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Monte Carlo estimators average a given function over these samples to approximate the expectation.

$$\frac{1}{N} \sum_{n=1}^{N} f(\theta_n) \sim \mathcal{N} \left( \mathbb{E}[f], \frac{\text{Var}[f]}{N} \right)$$
Usually we can’t generate exact samples from complex target distributions, but we can generate correlated samples.

\[ T(\theta \mid \theta') \]
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\[
\pi(\theta) = \int T(\theta \mid \theta') \pi(\theta') \, d\theta'
\]
A Markov transition that preserves the target distribution naturally concentrates towards the typical set.
Markov chains then provide a generic scheme for finding and then exploring the typical set.
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If run long the chain long enough then we can construct consistent Markov Chain Monte Carlo estimators.

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\[
\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N} f(\theta_n) \to \mathbb{E}[f]
\]
Unfortunately the performance of simple algorithms like Random Walk Metropolis does not scale well.
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In order to scale to high-dimensional target distributions we need a coherent exploration of the typical set.
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Approximations, such as data subsampling, perturb the typical set and frustrate accurate computation.
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Always be wary of approximations that require overlapping typical sets in high dimensions.
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