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1 import numpy as np
2
3
4 def split_r_hat(samples):
5     """
6     We take in samples, without the warm-up iterations, expecting an array of m chains by n iterations by
7     k estimands (parameters, variables, etc.). We then split each chain in the middle to arrive at 2m chains
8     of n/2 iterations each, on which we begin computing quantities. This all follows the logic detailed in
9     chapter 11 of Bayesian Data Analysis (Gelman et al., 2013).
10
11     :param samples: A numpy array of samples, as detailed above, m chains by n iterations by k parameters
12                     (estimands)
13     :return: The split  $\hat{R}$  statistic, an estimation of how much further scale reduction there might
14             be if the sampling was let to run with  $n \rightarrow \infty$  - optimally  $\hat{R} \approx 1$ 
15     """
16     marginal_posterior_variance, within_chain_variance = _marginal_posterior_variance(samples)
17     return np.sqrt(marginal_posterior_variance / within_chain_variance)
18
19
20 def _marginal_posterior_variance(samples):
21     """
22     Compute the marginal posterior variance as detailed leading up to equation (11.3) in Gelman (2016)
23     :param samples: A numpy array of samples, as detailed above, m chains by n iterations by k parameters
24                     (estimands)
25     :return: The marginal posterior variance  $\hat{\text{var}}(\phi \mid y)$ , as estimated by the within-chain
26             and between chain variances
27     """
28     m, n, k = samples.shape
29     split_chain_samples = np.vstack((samples[:, :n // 2, :], samples[:, n // 2:, :]))
30     m_eff, n_eff, _ = split_chain_samples.shape
31
32     per_chain_mean = np.mean(split_chain_samples, axis=1)
33     overall_mean = np.mean(per_chain_mean, axis=0)
34     between_chain_variance = n_eff / (m_eff - 1) * np.sum(np.square(per_chain_mean - overall_mean), axis=0)
35     per_chain_variance = 1 / (n_eff - 1) * np.sum(np.square(split_chain_samples - np.expand_dims(per_chain_mean, 1)),
36                                                    axis=1)
37     within_chain_variance = np.mean(per_chain_variance, axis=0)
38     marginal_posterior_variance = ((n_eff - 1) * within_chain_variance + between_chain_variance) / n_eff
39     return marginal_posterior_variance, within_chain_variance
40
41
42 def effective_sample_size(samples):
43     """
44     Estimate the effective sample sizes using the variograms (square difference at lag  $t$ ) to estimate
45     the autocorrelation at each lag  $t$ .
46
47     Interestingly, the code in PyStan looks substantially different than the algorithm descriptions
48     in the BDA textbook: https://github.com/stan-dev/pystan/blob/develop/pystan/\_chains.pyx starting
49     from the fact that their implementation is based on the autocovariance, rather than the autocorrelation
50
51     I tried to implement the code from the book, but the description is wholly incomplete. It is also
52     unclear how should one handle chains with different numbers of samples due to rejections.
53     :param samples: A numpy array of samples, as detailed above, m chains by n iterations by k parameters
54                     (estimands)
55     :return: An estimate of the effective sample size, ideally approaching the true number of samples taken.
56     """
57     marginal_posterior_variance, _ = _marginal_posterior_variance(samples)
58     m, n, k = samples.shape
59     split_chain_samples = np.vstack((samples[:, :n // 2, :], samples[:, n // 2:, :]))
60     m_eff, n_eff, _ = split_chain_samples.shape
61     # TODO: try centering the samples in each chain, inspired by the PyStan code
62     # note: this does nothing, except perhaps introduce numeric stability
63     split_chain_samples = split_chain_samples - np.expand_dims(np.mean(split_chain_samples, axis=1), 1)
64
65     # the stopping point for different variables might be different, which we need to account for
66     stopping_points = {}
67     t = 1
68     # TODO: unclear what to do if the correlation at lag one is negative - supposedly we would stop before it?
69     lag_correlations = [_estimate_lag_correlation(t, split_chain_samples, marginal_posterior_variance)]
70     while len(stopping_points) < k and t < (n_eff - 1):
71         rho_t_plus_1 = _estimate_lag_correlation(t + 1, split_chain_samples, marginal_posterior_variance)
72         rho_t_plus_2 = _estimate_lag_correlation(t + 2, split_chain_samples, marginal_posterior_variance)
73         lag_correlations.extend((rho_t_plus_1, rho_t_plus_2))
74
75         for i in range(k):
76             lag_correlation_sum = rho_t_plus_1[i] + rho_t_plus_2[i]
77             if i not in stopping_points and (lag_correlation_sum < 0):
78                 stopping_points[i] = t
79
80         t += 2
81
82     # verify we have a stopping point for every variable
83     # TODO: this might be where I deviate from Gelman - it's unclear if they set it to be
84     # TODO: the same for all variables, or independent for each one
85     for i in range(k):
86         if i not in stopping_points:
87             stopping_points[i] = len(lag_correlations)
88

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89     lag_correlations_array = np.asarray(lag_correlations).T
90     return np.asarray([m_eff * n_eff / (1 + 2 * np.sum(lag_correlations_array[i, :stopping_points[i]]))
91                        for i in range(k)])
92
93
94 def _estimate_lag_correlation(t, split_chain_samples, marginal_posterior_variance):
95     """
96     Estimate the autocorrelation at lag t using the variogram
97     :param t: The lag to estimate in
98     :param split_chain_samples: The samples for each chain, split in half, so double the actual
99     sampled chains but each with half the number of samples
100     :param marginal_posterior_variance: The marginal posterior variance estimated using the function
101     implemented above
102     :return: An estimate for the autocorrelation of the samples of each parameter (the third dimension
103     of the split_chain_samples parameter) using the variogram.
104     """
105     variogram = np.mean(np.square(split_chain_samples[:, t:, :] - split_chain_samples[:, :-1 * t, :]), axis=(0, 1))
106     return 1 - (variogram / (2 * marginal_posterior_variance))
```