We establish the equivalence between the boundedness of certain supremum operators and optimal spaces in Sobolev embeddings. We do this by exploiting known relations between higher-order Sobolev embeddings and isoperimetric inequalities. We provide an explicit way to compute both the optimal domain norm and the optimal target norm in a Sobolev embedding. Finally, we apply our results to higher-order Sobolev embeddings on John domains and on domains from the Maz'ya classes. Furthermore, our results are partially applicable to embeddings involving product probability spaces.