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A Laplace method for under-determined Bayesian optimal experimental designs

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Abstract

In Long et al. (2013), a new method based on the Laplace approximation was developed to accelerate the estimation of the post-experimental expected information gains (Kullback–Leibler divergence) in model parameters and predictive quantities of interest in the Bayesian framework. A closed-form asymptotic approximation of the inner integral and the order of the corresponding dominant error term were obtained in the cases where the parameters are determined by the experiment. In this work, we extend that method to the general case where the model parameters cannot be determined completely by the data from the proposed experiments. We carry out the Laplace approximations in the directions orthogonal to the null space of the Jacobian matrix of the data model with respect to the parameters, so that the information gain can be reduced to an integration against the marginal density of the transformed parameters that are not determined by the experiments. Furthermore, the expected information gain can be approximated by an integration over the prior, where the integrand is a function of the posterior covariance matrix projected over the aforementioned orthogonal directions. To deal with the issue of dimensionality in a complex problem, we use either Monte Carlo sampling or sparse quadratures for the integration over the prior probability density function, depending on the regularity of the integrand function. We demonstrate the accuracy, efficiency and robustness of the proposed method via several nonlinear under-determined test cases. They include the designs of the scalar parameter in a one dimensional cubic polynomial function with two unidentifiable parameters forming a linear manifold, and the boundary source locations for impedance tomography in a square domain, where the unknown parameter is the conductivity, which is represented as a random field.

MSC: 62K05; 65N21; 65C60

Keywords: Bayesian statistics; Optimal experimental design; Information gain; Laplace approximation; Monte Carlo sampling; Sparse quadrature

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Nomenclature

$\mathbf{1}_{\Omega_M}$	an indicator function that takes the value of 1 when $\boldsymbol{\theta} \in \Omega_M$, 0 otherwise
Δ_k	the length of the kth segment
$\boldsymbol{U}_h$	the nodal voltage vector
$h_p(\boldsymbol{s}, \boldsymbol{t})$	the logarithm of the prior weight function $p(\boldsymbol{s}, \boldsymbol{t})$ i.e., $log[p(\boldsymbol{s}, \boldsymbol{t})]$
$h(\boldsymbol{s}, \boldsymbol{t})$	the logarithm of posterior weight function, $p(\boldsymbol{s}, \boldsymbol{t}\vert\bar{\boldsymbol{y}})$ i.e., $\log[p(\boldsymbol{s}, \boldsymbol{t}\vert\bar{\boldsymbol{y}})]$
$\bar{\boldsymbol{y}} = \{y\}_{i=1}^{M}$	a set of observed data points
ϵ_Q	the prediction error
tr	the trace of a matrix
$\nabla_{\boldsymbol{s}}$	the gradient in $\boldsymbol{s}$
$\tilde{\boldsymbol{\Sigma}}_{\boldsymbol{s}\vert\boldsymbol{t}}$	the approximate conditional covariance matrix $\tilde{\boldsymbol{\Sigma}}_{\boldsymbol{s}\vert\boldsymbol{t}} = \frac{1}{M}\{\boldsymbol{U}^T[\boldsymbol{J}_g(\boldsymbol{f}(\hat{s}, \boldsymbol{t}))^T \boldsymbol{\Sigma}_{\epsilon}^{-1} \boldsymbol{J}_g(\boldsymbol{f}(\hat{s}, \boldsymbol{t}))]\boldsymbol{U}\}^{-1}$
$\mathbf{1}_{s=\hat{s}}$	an indicator function, which takes the value of 1 when $\boldsymbol{s} = \hat{s}$, and takes the value 0 otherwise
$\boldsymbol{E}_{\boldsymbol{s}}$	the sum of the data residuals, i.e., $\boldsymbol{E}_{\boldsymbol{s}} = \sum_{i=1}^{M} \boldsymbol{r}_i$
$\boldsymbol{F}_h$	the force vector
$\boldsymbol{H}_{\boldsymbol{g}}$	the Hessian of model $\boldsymbol{g}$ w.r.t. the parameter $\boldsymbol{\theta}$
$\boldsymbol{H}_{\boldsymbol{s}}$	the Hessian of model $\boldsymbol{g}$ w.r.t. the parameter $\boldsymbol{s}$
$\boldsymbol{J}_{\boldsymbol{g}}$	the Jacobian of model $\boldsymbol{g}$ w.r.t. the parameter $\boldsymbol{\theta}$
$\boldsymbol{J}_{\boldsymbol{s}}$	the Jacobian of $\boldsymbol{g}$ w.r.t. the parameter $\boldsymbol{s}$
$\boldsymbol{K}(\boldsymbol{\theta})$	the stiffness matrix
$\boldsymbol{n}$	the normal vector to the boundary
$\boldsymbol{r}_i$	the ith residual vector, i.e., $\boldsymbol{r}_i = \boldsymbol{g}(\boldsymbol{\theta}_0) + \epsilon_i - \boldsymbol{g}(\boldsymbol{\theta})$
$\boldsymbol{U}$	the matrix whose columns are the basis corresponding to the positive eigenvalues of $\boldsymbol{H}(\boldsymbol{f}(\mathbf{0}, \boldsymbol{t}))$
$\boldsymbol{V}$	the matrix whose columns are the basis corresponding to the zero eigenvalues of $\boldsymbol{H}(\boldsymbol{f}(\mathbf{0}, \boldsymbol{t}))$
$\boldsymbol{y}_i$	the ith $\boldsymbol{s} \times 1$ observable response vector
Λ	a diagonal matrix containing the eigenvalues of $\boldsymbol{H}(\boldsymbol{f}(\mathbf{0}, \boldsymbol{t}))$
$\boldsymbol{\xi}$	the $r \times 1$ vector of design parameters, also known as the experimental setup
$\boldsymbol{\epsilon}_1, \ldots, \boldsymbol{\epsilon}_M$	i.i.d. $s \times 1$ error vectors, with $\boldsymbol{\epsilon}_1 \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_{\epsilon})$
$\boldsymbol{\theta}_0$	the $d \times 1$ true parameter vector used to generate the synthetic data
a_j	the subset of the boundary corresponding to the jth electrode
d	the dimension of parameter vector $\boldsymbol{\theta}_0$
$d_{\boldsymbol{g}}$	the dimension of measurement vector $\boldsymbol{g}$
$H^1(\Omega)$	the Sobolev space with a square integrable gradient
$H_p(\hat{\boldsymbol{s}}, \boldsymbol{t})$	the Hessian of $h_p(\hat{s}, \boldsymbol{t})$
l	the total number of electrodes
M	the total number of observations
NQ	the number of quadrature points
$NS1$	the number of points in a one-dimensional mesh partitioning the domain of scalar Q
$O(\cdot)$	the big O notation
$O_P(\cdot)$	the big O in probability
$\mathbb{P}(\cdot)$	the probability measure
$p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$	the prior of the unknown random parameter $\boldsymbol{\theta}$
$p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}\vert\bar{\boldsymbol{y}})$	the posterior pdf of the unknown random parameter $\boldsymbol{\theta}$
$p_{\mathcal{Y}}(\bar{\boldsymbol{y}}\vert\boldsymbol{\xi})$	the Bayesian evidence, defined as the marginalization of likelihood over all admissible parameters
$p_{\boldsymbol{s}}(\mathbf{0}) = \int_{T_t} p(\mathbf{0}, \boldsymbol{t})dt$	the marginal of prior pdf of parameter $\boldsymbol{s}$
Q	the quantity of interest
U_j	the measured voltage on the jth electrode and part of the solution of the weak form of the Poisson equation
V_h	the finite element subspace of V, i.e., $V_h := \{v \in V : v$ is piecewise linear continuous over $\Omega_h\}$
w_i	the weights for the ith quadrature points
$\boldsymbol{g} : \mathbb{R}^d \times \mathbb{R}^k \to \mathbb{R}^s$	a deterministic nonlinear mapping