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#### Citation for published version:

Lung, R, Wu, Y, Kamilis, D & Polydorides, N 2020, 'A sketched finite element method for elliptic models', Computer Methods in Applied Mechanics and Engineering, vol. 364, 112933. https://doi.org/10.1016/j.cma.2020.112933

#### **Digital Object Identifier (DOI):**

10.1016/j.cma.2020.112933

#### Link:

Link to publication record in Edinburgh Research Explorer

**Document Version:** Peer reviewed version

**Published In:** Computer Methods in Applied Mechanics and Engineering

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### A sketched finite element method for elliptic models

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#### Abstract

We consider a sketched implementation of the finite element method for elliptic partial differential equations on high-dimensional models. Motivated by applications in real-time simulation and prediction we propose an algorithm that involves projecting the finite element solution onto a low-dimensional subspace and sketching the reduced equations using randomised sampling. We show that a sampling distribution based on the leverage scores of a tall matrix associated with the discrete Laplacian operator, can achieve nearly optimal performance and a significant speedup. We derive an expression of the complexity of the algorithm in terms of the number of samples that are necessary to meet an error tolerance specification with high probability, and an upper bound for the distance between the sketched and the highdimensional solutions. Our analysis shows that the projection not only reduces the dimension of the problem but also regularises the reduced system against sketching error. Our numerical simulations suggest speed improvements of two orders of magnitude in exchange for a small loss in the accuracy of the prediction.

*Keywords:* Randomised linear algebra, Galerkin finite element method, statistical leverage scores, real-time simulation. 2000 MSC: 65F05, 65M60, 68W20

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Preprint submitted to Computer Methods in Applied Mechanics and EngineeringFebruary 23, 2020

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<sup>&</sup>lt;sup>1</sup>RL acknowledges the support of the James Clerk Maxwell Foundation.

 $<sup>^{2}</sup>$ NP, YW and DK are grateful to EPSRC for funding this work through the grant EP/R041431/1, titled 'Randomness: a resource for real-time analytics'.

#### 1 1. Introduction

Motivated by applications in digital manufacturing twins and real-time 2 simulation in robotics, we consider the implementation of the Finite Ele-3 ment Method (FEM) in high-dimensional discrete models associated with elliptic partial differential equations (PDE). In particular, we focus on the 5 many-query context, where a stream of approximate solutions are sought for various PDE parameter fields [1], aiming to expedite computations in 7 situations where speedy model prediction is critical. Realising real-time 8 simulation with high-dimensional models is instrumental to enable digital 9 economy functions and has been driving developments in model reduction 10 over the last decade [2], including the popular and, in many cases, effective 11 Reduced-Basis method, which approximates the PDE solution manifold via 12 a low-dimensional reduced basis, built from solution snapshots using either 13 a POD or greedy construction [3, 4, 5]. Reducing the computational com-14 plexity of models is also central to the practical performance of statistical 15 inference and uncertainty quantification algorithms, where a multitude of 16 model evaluations are necessary to achieve convergence [6]. When real-time 17 prediction is coupled with noisy sensor data, as in the digital twins paradigm, 18 a fast, somewhat inaccurate model prediction typically suffices [7]. 19

Our approach is thus tailored to applications where some of the accuracy 20 of the solution can be traded off with speed. In these circumstances the 21 framework of randomised linear algebra presents a competitive alternative 22 [8]. In the seminal work [9], Drineas and Mahoney propose an algorithm 23 for computing the solution of the Laplacian of a graph, making the case for 24 sampling the rows of the matrices involved based on their statistical leverage 25 scores. Despite aimed explicitly for the symmetric diagonally dominant sys-26 tems arising in these problems, their approach provides inspiration for the 27 numerical solution of symmetric, positive definite and possibly ill-conditioned 28 systems originating from the discretisation of elliptic PDEs on unstructured 29 meshes. Apart from the algebraic resemblance to the Galerkin FEM systems, 30 the authors introduced sampling based on leverage scores of matrices through 31 the concept of 'effective resistance' of a graph derived by mimicking Ohmic 32 relations in resistor networks. As it turns out the complexity of computing 33 the leverage scores is similar to that of solving the high-dimensional prob-34 lem deterministically, however efficient methods to approximate them have 35

since been suggested [10]. More recently, Avron and Toledo have proposed an extension of [9] for preconditioning the FEM equations by introducing the 'effective stiffness' of an element in a finite element mesh [11]. Specifically, for sparse symmetric positive definite (SSPD) stiffness matrices, they derive an expression for the effective stiffness of an element and show its equivalence to the statistical leverage scores. Sampling  $O(n \log n)$  elements leads to a sparser preconditioner.

In situations where a single, high-dimensional linear system is sought, 43 randomised algorithms suited to SSPD systems are readily available. The 44 methods of Gower and Richtarik for example randomises the row-action iter-45 ative methods by taking a sequence of random projections onto convex sets 46 [12]. This algorithm is equivalent to a stochastic gradient descent method 47 with provable convergence, while their alternative approach in [13] iteratively 48 sketches the inverse of the matrix. In [14], Bertsekas and Yu present a Monte 40 Carlo method for simulating approximate solutions to linear fixed-point equa-50 tions, arising in evaluating the cost of stationary policies in Markovian deci-51 sions. Their algorithm is based on approximate dynamic programming and 52 has subsequently led to [15], that extends some of the proposed importance 53 sampling ideas in the context of linear ill-posed inverse problems. 54

Real-time FEM computing at the many query paradigm, is hindered by 55 two fundamental challenges: the fast assembly of the stiffness matrix for each 56 parameter field, unless the domain consists of a small number of regions with 57 homogeneous isotropic materials, and the efficient solution of the resulting 58 system to the required accuracy. To mitigate these, is to compromise slightly 59 on the accuracy in order to capitalise on speed. To achieve this we first trans-60 form the linear SSPD system into an overdetermined least squares problem, 61 and then project its solution this onto a low-dimensional subspace. This 62 mounts to inverting a low-dimensional, dense matrix whose entries are per-63 turbed by random errors. Our emphasis and contributions are in developing 64 the projected sketching algorithm, and in optimising the sampling process so 65 that it is both efficient in the multi-query context and effective in suppressing 66 the variance of the solution. We also analyse the complexity of our algorithm 67 and derive, probabilistic error bounds for quality of the approximation. 68

Our paper is organised as follows: In section 2 we provide a concise introduction to the Galerkin formulation for elliptic boundary value problems, and subsequently derive the projected least squares formulation of the problem. We then describe the sampling distribution used in the sketching and provide the conditions under which the reduced sketched system has a unique solution. Section 4 contains a description of our algorithm, and our main result
that describes the complexity of our algorithm in achieving an error tolerance
in high probability. We then provide an error analysis addressing the various
types of errors imparted on the solution through the various stages of the
methodology, before concluding with some numerical experiments based on
the steady-state diffusion equation.

#### 80 1.1. Notation

Let [m] denote the set of integers between 1 and m inclusive. For a matrix 81  $X \in \mathbb{R}^{m \times n}$ ,  $X_{(\ell)}$  and  $X^{(\ell)}$  denote its  $\ell$ -th row and column respectively, and 82  $X_{ij}$  its (i, j)-th entry.  $X^{\dagger}$  is the pseudo-inverse of X and  $\kappa(X)$  its condition 83 number. If  $m \ge n$  we define the singular value decomposition  $X = U_X \Sigma_X V_X^T$ 84 where  $U_X \in \mathbb{R}^{m \times n}$ ,  $\Sigma_X \in \mathbb{R}^{n \times n}$  and  $V_X \in \mathbb{R}^{n \times n}$ . Notice that the form 85 of the SVD used in this work is the more economical reduced/thin variant 86 where the matrix  $U_X$  is not square and due to  $n \leq m$  the matrix  $\Sigma_X$  is 87 invertible whenever X has full column rank. Unless stated otherwise, singular 88 values and eigenvalues are ordered in non-increasing order. Analogously, for 80 a symmetric and positive definite matrix  $A \in \mathbb{R}^{m \times m}$ ,  $\lambda_{\max(A)}$  is the largest 90 eigenvalue, and  $\lambda_{\min(A)}$  the smallest. By  $\operatorname{nnz}(A)$  we denote the number of 91 non-zero elements in A. Further we write  $\|\cdot\|$  for the Euclidean norm for a 92 vector or the spectral norm of a matrix and  $\|\cdot\|_F$  the Frobenius norm of a 93 matrix. For matrices X and Y with the same number of rows (X|Y) is the 94 augmented matrix formed by column concatenation. The identity matrix is 95 expressed as I or  $I_n$  to specify its dimension n when important to the context. 96 We write  $y \otimes 1_n$  for the Kronecker product of vector y with the ones vector 97 in n dimensions. 98

#### <sup>99</sup> 2. Galerkin finite element method preliminaries

<sup>100</sup> Consider the elliptic partial differential equation

$$-\nabla \cdot p \nabla u = f \quad \text{in} \quad \Omega, \tag{1}$$

on a bounded, simply connected domain  $\Omega \subset \mathbb{R}^d$ ,  $d \in \{2,3\}$  with Dirichlet conditions

$$u = g^{(D)} \quad \text{on} \quad \partial\Omega, \tag{2}$$

<sup>103</sup> on a Lipschitz smooth boundary  $\partial \Omega$  for a sufficiently smooth function  $g^{(D)}$ . <sup>104</sup> Further let p a bounded positive parameter function in the Banach space 105  $L^{\infty}(\Omega)$  such that

$$0 < p_{\min} \le p \le p_{\max} < \infty \quad \text{on} \quad \Omega \cup \partial\Omega, \tag{3}$$

If we consider  $\mathcal{T}_{\Omega} \doteq \{\Omega_1, \dots, \Omega_k\}$  a mesh comprising k elements, having n interior and  $n_{\partial}$  boundary vertices (nodes) and

$$\mathcal{S}_{\Omega}^{1} \doteq \operatorname{span}\{\phi_{1}, \ldots, \phi_{n}, \ldots, \phi_{n+n_{\partial}}\}$$

to comprise linear interpolation shape functions with local support over the elements in  $\mathcal{T}_{\Omega}$  then the weak form of (1), see [16] chapter 6, can be discretised to yield the Galerkin system of equations for the vector  $\{u_1, \ldots, u_n\}$  and each  $i = 1, \ldots, n$ 

$$\sum_{j=1}^{n} \left( \sum_{\Omega_{\ell} \in \mathcal{T}_{\Omega}} \int_{\Omega_{\ell}} \mathrm{d}x \, \nabla \phi_{i} \cdot p_{\ell} \nabla \phi_{j} \right) u_{j} = \sum_{\Omega_{\ell} \in \mathcal{T}_{\Omega}} \int_{\Omega_{\ell}} \mathrm{d}x \, f_{\ell} \phi_{i} - \sum_{j=n+1}^{n+n_{\partial}} \left( \sum_{\Omega_{\ell} \in \mathcal{T}_{\Omega}} \int_{\Omega_{\ell}} \mathrm{d}x \nabla \phi_{i} \cdot p_{\ell} \nabla \phi_{j} \right) u_{j}.$$

$$(4)$$

 $_{106}$  At the same time (2) gives the boundary conditions of the form

$$u_j = g_j, \qquad j = n + 1, \dots, n_\partial \tag{5}$$

with  $g_j$  given by evaluating the boundary function  $g^{(D)}$  at the *j*-th node. The coefficients in the above equation are defined as the element-average coefficients

$$p_{\ell} = \frac{1}{|\Omega_{\ell}|} \int_{\Omega_{\ell}} \mathrm{d}x \, p, \quad \text{and} \quad f_{\ell} = \frac{1}{|\Omega_{\ell}|} \int_{\Omega_{\ell}} \mathrm{d}x \, f, \quad \ell = 1, \dots, k \tag{6}$$

which correspond to the piecewise constant approximations of the parameter and forcing term. The linear equations in (4) and (5) are expressed in a matrix form as

$$Au = b, (7)$$

where  $A \in \mathbb{R}^{n \times n}$  is the symmetric, sparse and positive-definite stiffness ma-113 trix, whose dependence on the parameters p is implicit and suppressed for 114 clarity. The FEM construction guarantees the consistency of the system (7), 115 thus  $b \in \mathbb{R}^n$  is always in the column space of A and consequently it admits 116 a unique solution  $u_{\text{opt}} = A^{-1}b$ . As we focus to the efficient approximation of 117  $u_{\rm opt}$  in the many query context we content with two challenges: the efficient 118 assembly of the stiffness matrix, and the speedy solution of the resulted FEM 119 system. 120

#### 121 2.1. The stiffness matrix

Let  $\mathcal{I}_{\ell}$  be the index set of the d+1 vertices of the  $\ell$ th element, and consider  $D_{\ell} \in \mathbb{R}^{d \times n}$  to be the sparse matrix holding the gradients of the linear shape functions  $\phi_i$  where  $i \in \mathcal{I}_{\ell}$ . In this  $D_{\ell}^{(i)}$  is then a constant gradients vector associated with the *i*th node of  $\Omega_{\ell}$ , and let  $z_{\ell} = |\Omega_{\ell}| p_{\ell}$  the element of a vector  $z \in \mathbb{R}^k$  such that  $Z^2 = \text{diag}(z \otimes 1_d)$  and  $D \in \mathbb{R}^{kd \times n}$  a row concatenation of  $D_{\ell}$  matrices for all elements. If we define as  $Y_{\ell} = \sqrt{z_{\ell}} D_{\ell}$  and  $Y \in \mathbb{R}^{kd \times n}$  the concatenation of the  $Y_{\ell}$  matrices as

$$Y = ZD \tag{8}$$

then the stiffness matrix takes the form of a high-dimensional sum or product
 of sparse matrices

$$A = \sum_{\ell=1}^{k} Y_{\ell}^{T} Y_{\ell} = Y^{T} Y.$$
 (9)

The above construction typically leads to a stiffness matrix that is wellconditioned for inversion with the exception of acute element skewness [17] and parameter vectors with wild variation [18], which cause the condition number  $\kappa(A)$  to increase dramatically. Explicit bounds on the largest and smallest eigenvalues of A, and respectively the singular values of Y, are given in [19].

#### <sup>137</sup> 3. A regularised sketched formulation

Broadly speaking, the randomised sketching technique [8] provides a rigorous framework for speeding up numerical linear algebra operations, such as regression or low-rank approximation problems, at the cost of introducing a provably controllable error. This is achieved by compressing high dimensional vectors or matrices to a much smaller size by multiplying them by a random sketching matrix S. The matrix S should ideally be such that for a high dimensional quantity Y, i.e. a large matrix or vector,

- $\hat{Y} = S^T Y$  can be computed (substantially) faster than the solution to the original un-sketched problem and
- $\hat{Y}$  is a good enough approximation of Y in a way specific to the problem at hand.

The first criterion is very simple and ensures that computing the sketch isn't 149 prohibitively expensive. The second criterion should be understood in terms 150 of the solution x of the original problem which often involves some form of 151 optimisation. More specifically, an  $\varepsilon$ -accurate sketch  $\hat{Y}$  of Y for finding an 152 approximate solution  $\hat{x}$  ensures that  $\|\hat{x} - x\| \leq \varepsilon \|x\|$ . In other words, the 153 sketched matrix is a good approximation of its high-dimensional counterpart 154 if it can be used to solve the problem of interest subject to a small relative 155 error. The acceleration from sketched methods consequently scales with the 156 amount of compression that can be applied to Y while keeping the error 157 acceptable. 158

In the case of linear regression problems, good computational gains can 159 usually be expected when the matrices that should be sketched have signif-160 icantly more rows than columns and the resulting systems are highly over-161 determined. Intuitively this observation can be explained by noticing that 162 there is a certain amount of redundancy in an over-determined system and 163 thus there is some hope that it can be compressed and solved more efficiently. 164 In order to understand how this technique can be applied in our context we 165 start by observing that the sought solution  $u_{opt} = A^{-1}b$  can be alternatively 166 obtained by solving the over-determined least squares problem 167

$$u_{\text{opt}} = u_{\text{LS}} = \arg\min_{u \in \mathbb{R}^n} \|Yu - (Y^T)^{\dagger}b\|^2,$$
 (10)

since

$$u_{\rm LS} = (Y^T Y)^{-1} Y^T (Y^T)^{\dagger} b = A^{-1} Y^T (Y^T)^{\dagger} b = A^{-1} b = u_{\rm opt}.$$

The fact that the above problem is over-determined implies, at least to some extent, robustness against noise, such as random perturbations on the elements of the matrix Y and vector b. A similar error is induced by randomised sketching where we replace (10) with

$$\hat{u}_{\text{LS}} = \arg\min_{u \in \mathbb{R}^n} \|\hat{Y}u - (\hat{Y}^T)^{\dagger}b\|^2,$$
 (11)

and look for a random approximation  $\hat{Y}$  of Y in the sense that  $\hat{u}_{\text{LS}} \approx u_{\text{LS}}$ . We note that  $\hat{Y}$  and Y don't have to be similar as such, e.g. have the same dimensions, as long as the problems are well defined and the optimisers remain similar. Following [9] and [20] we seek to approximate Y with some sketch  $\hat{Y}$  by sampling and scaling rows according to probabilities that will be specified later. The number of rows in  $\hat{Y}$  in that case equals the number of drawn samples. Clearly  $\hat{Y}$  must have at least n rows as otherwise the problem (11) will be under-determined and, due to the non-uniqueness of the solution, the error could become arbitrarily large. On the other hand, if around  $n \log(n)$  rows are sampled from a suitable distribution, then Drineas and Mahoney [9] show that the resulting sketch is a good approximation with high probability. However, if substantially less than  $n \log(n)$  samples are drawn then the sketching induced error outweighs its computational benefits. In order to understand how this issue can be addressed we note that, if  $\hat{Y}$  has full column-rank and thus the optimiser of (11) is unique, the solution of the sketched problem can be obtained by solving the linear system

$$\hat{Y}^T \hat{Y} u = b$$

<sup>172</sup> which is equivalent to solving

$$Y^{T}Yu = b + (Y^{T}Y(\hat{Y}^{T}\hat{Y})^{-1} - I)b = \hat{b}.$$
(12)

From (12) it becomes clear that the sketching induced error can be regarded as an error on the right-hand side of the linear system (7) or the least squares problem (10). We can easily obtain a bound for the relative error given by

$$\frac{\|\hat{b} - b\|}{\|b\|} \le \|Y^T Y(\hat{Y}^T \hat{Y})^{-1} - I\|$$

A standard way of dealing with noise as in (12) is regularisation [21]. Suppose that there exists a low-dimensional subspace

$$\mathcal{S}_{\rho} \doteq \{ \Psi r \,|\, r \in \mathbb{R}^{\rho} \},\tag{13}$$

spanned by a basis of  $\rho \ll n$  orthonormal functions arranged in the columns 175 of matrix  $\Psi$ , and assume that is sufficient to approximate  $u_{opt}$  within some 176 acceptable level of accuracy, in the sense of incurring a small subspace error 177  $\|(I - \Pi)u_{\text{opt}}\|$ . The orthogonal projection operator  $\Pi \doteq \Psi \Psi^T$  maps vectors 178 from  $\mathbb{R}^n$  onto the subspace  $\mathcal{S}_{\rho}$ . Of course, such a subspace can't accommodate 179 all but rather only sufficiently regular  $u \in \mathbb{R}^n$ . For that reason  $\mathcal{S}_{\rho}$  has to be 180 constructed using prior information (e.g. degree of smoothness) about the 181 solution. Orthogonality of  $\Psi$  ensures for any  $u_{\text{opt}} = \Pi u_{\text{opt}} + (I - \Pi) u_{\text{opt}}$  the 182 existence of a unique, optimal low-dimensional vector  $r_{\rm opt}$  satisfying 183

$$\Psi r_{\rm opt} = \Pi u_{\rm opt}.\tag{14}$$

<sup>184</sup> In these conditions we can pose a projected-regularised least-squares problem <sup>185</sup> replacing (10) by

$$\Pi u_{\text{opt}} \approx u_{\text{reg}} = \arg \min_{u \in \mathcal{S}_{\rho}} \|Yu - (Y^T)^{\dagger}b\|^2,$$
(15)

<sup>186</sup> in order to improve the robustness of the solution against sketching-induced <sup>187</sup> errors. The problem in (15) still involves high-dimensional quantities such <sup>188</sup> as Y and b, but the solution is unique as soon as  $S_{\rho}$  and the null-space of Y <sup>189</sup> have {0} intersection. We start by introducing the low dimensional problem<sup>3</sup> <sup>190</sup>

$$r_{\text{reg}} = \arg\min_{r \in \mathbb{R}^{\rho}} \|Y\Psi r - (Y^T)^{\dagger}b\|^2.$$
(16)

<sup>191</sup> A solution  $r_{\text{reg}}$  of (16) yields a solution  $u_{\text{reg}} = \Psi r_{\text{reg}}$  of (15) because the <sup>192</sup> columns of  $\Psi$  form an orthonormal basis (ONB) of its column-space  $S_{\rho}$  by <sup>193</sup> construction. In addition, we have the following.

Lemma 3.1. If Y has full column rank and the columns of  $\Psi$  form an ONB of  $S_{\rho}$  so that  $\Pi = \Psi \Psi^{T}$  is the projection onto  $S_{\rho}$ , then

$$\arg\min_{u\in\mathcal{S}_{\rho}} \|Yu - (Y^{T})^{\dagger}b\|^{2} = \arg\min_{u\in\mathcal{S}_{\rho}} \|Y\Pi u - (\Psi^{T}Y^{T})^{\dagger}\Psi^{T}b\|^{2}.$$
 (17)

### <sup>196</sup> In particular, both problems have a unique solution.

*Proof.* Both problems have unique solutions because  $S_{\rho}$  is convex and Y has (by assumption) full column rank. Therefore it suffices to show that there exists an element  $u_{\text{reg}} \in S_{\rho}$  that solves both problems. The solution  $r_{\text{reg}}$  of (16) can be found explicitly by solving the linear system

$$\Psi^T Y^T Y \Psi r = \Psi^T Y^T (Y^T)^{\dagger} b \iff r_{\text{reg}} = (\Psi^T Y^T Y \Psi)^{-1} \Psi^T b.$$

$$r' = \arg\min_{r \in \mathbb{R}^{\rho}} \left\| A\Psi r - b \right\|^2,$$

whose solution is

$$r' = (\Psi^T A^2 \Psi)^{-1} \Psi^T A b = \Psi^T u + (\Psi^T A^2 \Psi)^{-1} \Psi^T A^2 (I - \Pi) u_{\underline{v}}$$

and incurs a subspace regression error term that is quadratic in A. Moreover, note that the right hand side vector in the normal equations  $\Psi^T A^T A \Psi r' = \Psi^T A^T b$  has dependence on the parameter through A.

<sup>&</sup>lt;sup>3</sup>We emphasise the contrast between the projected equations in (16) and the projected variable least squares problem

We have used that Y has full column rank so that  $Y^T(Y^T)^{\dagger} = I$  and  $\Psi^T Y^T Y \Psi$  is invertible. Similarly we may consider

$$\arg\min_{r\in\mathbb{R}^{\rho}}\|Y\Pi\Psi r - (\Psi^T Y^T)^{\dagger}\Psi^T b\|^2,$$

which produces solutions  $r_{\Psi}$  such that  $\Psi r_{\Psi}$  is a solution of the right-hand side of (17). Since  $\Pi \Psi = \Psi$  and  $Y \Psi$  has full column rank we can write  $r_{\Psi}$  as

$$\Psi^T Y^T Y \Psi r_{\Psi} = \Psi^T Y^T (\Psi^T Y^T)^{\dagger} \Psi^T b \iff r_{\Psi} = (\Psi^T Y^T Y \Psi)^{-1} \Psi^T b.$$

<sup>197</sup> We conclude that  $\Psi(\Psi^T Y^T Y \Psi)^{-1} \Psi^T b$  is a solution to both sides of (17) which <sup>198</sup> completes the proof.

<sup>199</sup> The right hand side of (17) has a very natural interpretation and is ob-<sup>200</sup> tained by embedding the rows of Y, the vector b and the variable u in  $S_{\rho}$  using <sup>201</sup> its low dimensional representation from the basis induced by the columns of <sup>202</sup>  $\Psi$ . In view of Lemma 3.1 we may regularise the problem from (11) and obtain <sup>203</sup> an embedded sketched counterpart to (15) as

$$\hat{u}_{\text{reg}} = \arg\min_{u\in\mathcal{S}_{\rho}} \|\hat{Y}\Pi u - (\Psi^T \hat{Y}^T)^{\dagger} \Psi^T b\|^2.$$
(18)

We argue that (18) is much more robust to the noise imparted by the approximation  $\hat{Y}$  and produces solutions with controlled errors even if substantially less than *n* suitably drawn samples are used for the approximation. In order to see why, notice that the problem (18) can be expressed in terms of the low-dimensional vector of coefficients

$$\hat{r}_{\text{reg}} = \arg\min_{r \in \mathbb{R}^{\rho}} \|\hat{Y}\Psi r - (\Psi^T \hat{Y}^T)^{\dagger} \Psi^T b\|^2.$$
(19)

so that  $\Psi \hat{r}_{reg} = \hat{u}_{reg}$ . Recalling that  $A = Y^T Y$ , it is convenient to introduce

$$X = Y\Psi \quad \text{and} \quad G = X^T X = \Psi^T A\Psi, \tag{20}$$

<sup>210</sup> together with their sketched approximations

$$\hat{X} = \hat{Y}\Psi$$
 and  $\hat{G} = \hat{X}^T\hat{X}$ . (21)

Lemma 3.2. If  $\hat{X} = \hat{Y}\Psi$  has full column rank then the solution of the leastsquares problem (19) is given by  $\hat{r}_{reg} = \hat{G}^{-1}\Psi^T b$  and we have

$$\hat{u}_{\rm reg} = \Psi \hat{r}_{\rm reg} = u_{\rm reg} + \Psi (\hat{G}^{-1}G - I)\Psi^T u_{\rm reg}.$$
(22)

<sup>213</sup> where  $u_{\text{reg}}$  and  $\hat{u}_{\text{reg}}$  are the solutions of (15) and (18) respectively.

*Proof.* If  $\hat{Y}\Psi$  has linearly independent columns then  $\Psi^T \hat{Y}^T (\Psi^T \hat{Y}^T)^{\dagger} = I$  and the solution  $\hat{r}_{reg}$  of (19) solves

$$\hat{G}r = \Psi^T b.$$

Again  $\hat{G}$  is invertible because  $\hat{Y}\Psi$  has linearly independent columns and the first claim follows. The matrix A is positive definite which implies that G is positive definite and  $u_{\text{reg}} = \Psi G^{-1} \Psi^T b$ . The matrix  $\Psi$  has orthonormal columns which implies  $\Psi^T b = G \Psi^T u_{\text{reg}}$ . Since  $\hat{u}_{\text{reg}} = \Psi \hat{r}_{\text{reg}}$  we can use the formula we have just shown and obtain

$$\begin{split} \hat{u}_{\mathrm{reg}} &= \Psi \hat{r}_{\mathrm{reg}} \\ &= \Psi \hat{G}^{-1} \Psi^T b \\ &= \Psi \hat{G}^{-1} G \Psi^T u_{\mathrm{reg}} \\ &= \Psi \hat{G}^{-1} (\hat{G} + (G - \hat{G})) \Psi^T u_{\mathrm{reg}} \\ &= \Pi u_{\mathrm{reg}} + \Psi (\hat{G}^{-1} G - I) \Psi^T u_{\mathrm{reg}} \\ &= u_{\mathrm{reg}} + \Psi (\hat{G}^{-1} G - I) \Psi^T u_{\mathrm{reg}} \end{split}$$

where the last identity is due to  $u_{\text{reg}} \in \mathcal{S}_{\rho}$ .

In order to understand the effect of row sampling and why it can be a good approximation, recall that k is the number of elements and d the dimension, we can start by writing

$$G = \sum_{j=1}^{kd} X_{(j)}^T X_{(j)} = X^T X \quad \text{and} \quad A = \sum_{j=1}^{kd} Y_{(j)}^T Y_{(j)} = Y^T Y$$
(23)

as a sum of outer products of rows. Introduce for some sample size  $c \in \mathbb{N}$ the iid random indices  $\mathbf{i}_1, \ldots, \mathbf{i}_c$  taking values in [kd] with distribution

$$\mathbb{P}(\mathbf{i}_j = i) = q_i \tag{24}$$

for each  $j \in [c]$  and  $i \in [kd]$ . Instead of (23) we may consider the sketch

$$\hat{G} = \frac{1}{c} \sum_{j=1}^{c} \frac{1}{q_{\mathbf{i}_j}} X_{(\mathbf{i}_j)}^T X_{(\mathbf{i}_j)}.$$
(25)

If we define the random matrix  $R \in \mathbb{R}^{kd \times c}$  and the random diagonal matrix  $W \in \mathbb{R}^{c \times c}$  via

$$R_{ij} = \begin{cases} 1 & \text{if } \mathbf{i}_j = i \\ 0 & \text{if } \mathbf{i}_j \neq i \end{cases}, \qquad W_{jj} = \frac{1}{\sqrt{cq_{\mathbf{i}_j}}}, \tag{26}$$

<sup>223</sup> then can put S = RW and construct the sketch  $\hat{G}$  as

$$\hat{G} = X^T S S^T X = X^T R W^2 R^T X.$$
(27)

Lastly, we can write  $\hat{Y} = S^T Y$  as well as  $\hat{X} = \hat{Y} \Psi = S^T Y \Psi$  for the sketches of Y and X. A simple computation together with an application of the strong law of large numbers shows the following.

Proposition 3.3 (Lemma 3 and 4 in [22]). Assume that the sampling probabilities satisfy the consistency condition

$$X_{(j)} \neq 0 \implies q_j > 0 \qquad \forall j = 1, \dots, kd.$$
 (28)

In this case we have for the matrix  $\hat{G}$  as defined in (25) that  $\mathbb{E}[\hat{G}] = G$  and  $\mathbb{E}[\|\hat{G} - G\|_F^2] = \mathcal{O}(c^{-1})$ . As a consequence,  $\hat{G} \to G$  almost surely for  $c \to \infty$ .

Proposition 3.3 summarises the asymptotic properties of the used sketch. 231 The condition (28) is very mild and holds for a wide range of distributions 232 such as sampling from scaled row norms or uniform sampling. The con-233 vergence rate of  $c^{-1}$  cannot be improved although the constant depends on 234 the chosen probabilities  $q_i$ . In other words, as long as we sample all non-235 zero rows with positive probability we will obtain a sketch that has good 236 asymptotic properties when considered as an approximation for G. How-237 ever, in order to find good sampling probabilities  $q_i$  we have to consider the 238 non-asymptotic behaviour of the sketch. In fact, the main purpose of the reg-239 ularisation/dimensionality reduction was to avoid situations where sampling 240 a large number of rows is necessary. If  $\rho \ll n$ , then the regularised problem 241 (16) has substantially fewer degrees of freedom than the high dimensional 242 formulation in (10). Consequently, the dependence of G on the rows of X243 is a lot smoother than the dependence of A on  $Y_{(i)}$ . In other words, ap-244 proximating X by row sampling has a much smaller effect on the regularised 245 solution  $u_{reg}$  than an approximation of Y with the same sample size c would 246 have on the solution u of the full system (7). For example, a much smaller 247

number of rows needs to be sampled to obtain the correct null-space which results in a full-rank approximation of G. Note that, conditional on  $\hat{G}$  being invertible,  $u_{\text{reg}} \in S_{\rho}$  in combination with Lemma 3.2 implies

$$\frac{\|u_{\text{reg}} - \hat{u}_{\text{reg}}\|}{\|u_{\text{reg}}\|} \le \|\hat{G}^{-1}G - I\|,$$
(29)

so the randomisation error of the regularised problem is entirely controlled by low dimensional structures. This property is the key to a small sketching error and thus to an overall accurate approximation when only few samples are drawn. Using the notation from before and letting  $X = U_X \Sigma_X V_X^T$  be the singular value decomposition of X, we can write the bound from (29) as

$$\|\hat{G}^{-1}G - I\| = \|\Sigma_X^{-1}(U_X^T S S^T U_X)^{-1} \Sigma_X - I\|.$$

From the above formulation it becomes apparent that the error will be small if the sketch is constructed such that  $(U_X S S^T U_X)^{-1} \approx I$  in spectral norm.

We argue that this is essentially equivalent to  $U_X SS^T U_X \approx I$ . Indeed, we have the following.

Lemma 3.4. If 
$$||U_X^T S S^T U_X - I|| < \varepsilon < 1$$
 then  
 $1 - \varepsilon \le \frac{||U_X^T S S^T U_X - I||}{||(U_X^T S S^T U_X)^{-1} - I||} \le 1 + \varepsilon.$ 

*Proof.* Under the condition of the lemma we know that  $U_X S S^T U_X$  is invertible and that

$$||U_X^T S S^T U_X|| \le ||I|| + ||U_X^T S S^T U_X - I|| < 1 + \varepsilon$$

which implies the upper bound by considering the estimate

$$||U_X^T S S^T U_X - I|| \le ||U_X^T S S^T U_X|| ||(U_X^T S S^T U_X)^{-1} - I|| \le (1 + \varepsilon) ||(U_X^T S S^T U_X)^{-1} - I||.$$

Denote by  $\lambda_i(U_X S S^T U_X)$  the *i*-th eigenvalue of  $U_X S S^T U_X$ . Then we may write

$$\| (U_X S S^T U_X)^{-1} - I \| = \max_{i=1}^{\rho} |1 - \lambda_i^{-1} (U_X^T S S^T U_X)|$$
  
$$= \max_{i=1}^{\rho} \frac{|1 - \lambda_i (U_X^T S S^T U_X)|}{\lambda_i (U_X^T S S^T U_X)}$$
  
$$\leq \frac{\|1 - U_X^T S S^T U_X\|}{\lambda_{\min} (U_X^T S S^T U_X)}$$

where  $\lambda_{\min}(U_X S S^T U_X)$  is the smallest eigenvalue. By assumption of the lemma

$$|1 - \lambda_{\min}(U_X^T S S^T U_X)| \le \varepsilon \implies \lambda_{\min}(U_X^T S S^T U_X) \ge 1 - \varepsilon$$

which implies the claim after dividing by  $||1 - U_X^T S S^T U_X||$  and taking the inverse.

An approximation of  $U_X^T S S^T U_X$  can be obtained by sampling with probabilities that are proportional to the statistical leverage scores

$$\ell_i(X) = \ell_i(U_X) = \|(U_X)_{(i)}\|^2, \tag{30}$$

i.e. the row norms of the left singular vectors of X [10]. At first sight it seems 259 that taking sampling probabilities proportional to the leverage scores in (30)260 in order to obtain a sketch of (16) is very similar to using the leverage scores 261 of Y to obtain (11) from (10) as was proposed by Drineas and Mahoney in 262 [9] for a similar problem. A key difference is that X is tall and dense while 263 Y is sparse and thus G is quite different to the initial stiffness matrix A. 264 Consequently, an interpretation of the leverage scores from (30) in terms of 265 effective stiffness [11] is, to the best of our knowledge, not possible. The 266 following Lemma will be useful for our further developments. 267

Lemma 3.5 ([23] section 6.4). Assume that S is constructed as before with sampling probabilities  $q_i$  satisfying

$$q_i \ge \beta \frac{\ell_i(X)}{\rho} \quad i = 1, \dots, kd \tag{31}$$

270 for some  $\beta \in (0,1]$ . Then we have  $\forall \varepsilon > 0$ 

$$\mathbb{P}\left(\|U_X^T S S^T U_X - I\| \ge \varepsilon\right) \le 2\rho \exp\left(-\frac{3c\beta\varepsilon^2}{12\rho + 4\rho\varepsilon}\right)$$
(32)

An important corollary of the above lemma is that a sketch which is constructed by sampling from leverage score probabilities will virtually always be invertible and therefore the sketched problem (19) has a unique solution. The following result states that this property is preserved even when the rows are re-weighted, an operation which changes the leverage scores. **Proposition 3.6.** Let  $\Gamma \in \mathbb{R}^{kd \times kd}$  be a diagonal matrix with positive entries, *i.e.*  $\Gamma_{ii} > 0$  for each i = 1, ..., kd. Assume that the sketching matrix S is constructed with sampling probabilities  $q_i = \rho^{-1}\ell_i(X)$ . For the scaled sketch  $\hat{H} = X^T \Gamma S S^T \Gamma X$  we have

$$\mathbb{P}(\hat{H} \text{ is invertible}) = \mathbb{P}(\hat{G} \text{ is invertible}) \ge 1 - 2\rho \exp\left(-\frac{3c}{16\rho}\right)$$
(33)

*Proof.* It is sufficient to show that

 $\hat{H}$  is invertible  $\iff \hat{G}$  is invertible  $\iff U_X^T S S^T U_X$  is invertible

because the probability bound follows immediately from

$$\mathbb{P}(U_X^T S S^T U_X \text{ is invertible}) \ge 1 - \mathbb{P}\left( \|U_X^T S S^T U_X - I\| \ge 1 \right)$$

after applying (32) from Lemma 3.5. The above matrices are always positive semi-definite and therefore invertibility is equivalent to positive definiteness. For any diagonal matrix  $\Gamma$  it holds that  $S^T\Gamma = \hat{\Gamma}S^T$  where  $\hat{\Gamma}$  is a random diagonal matrix with entries  $\hat{\Gamma}_{ij} = \Gamma_{i_j i_j}$ . Thus for any  $x \in \mathbb{R}^{\rho}$  we have

$$x^T \hat{H} x = (\Sigma_X V_X^T x)^T U_X^T S \hat{\Gamma}^2 S^T U_X (\Sigma_X V_X^T x).$$

Since X has full column rank we know that  $\Sigma_X V_X^T$  corresponds to a change of basis and  $\Sigma_X V_X^T x \neq 0$  whenever  $x \neq 0$ . It follows that  $\hat{H}$  is positive definite if and only if  $U_X^T S \hat{\Gamma}^2 S^T U_X$  is positive definite. As  $\hat{\Gamma}$  is a diagonal such that  $\hat{\Gamma}_{jj} > 0$  with probability 1, the latter is equivalent to  $U_X^T S S^T U_X$ being positive definite. The case of  $\hat{G}$  is covered by  $\Gamma = I$ .

Proposition 3.6 states that re-scaling of rows doesn't affect the quality of 285 the sketching matrix regarding its invertibility and after sampling  $\rho \log(\rho)$ 286 rows the probability of the sketch being singular decays exponentially fast 287 with each additional draw. In practice this makes knowledge of  $\ell_i(X)$  valu-288 able because we only need to sample  $\rho \log(\rho) + M$  rows for some moderately 289 large M and obtain a sketch that is virtually never singular. On the other 290 hand, we need at least  $\rho$  samples so that there is any hope in obtaining a 291 non-singular matrix. The remarkable thing about Proposition 3.6 is that 292 the failure probability is *independent* of both, the inner dimension kd of the 293 product  $X^T X$  as well as the scaling matrix  $\Gamma$  and equivalent to the bound 294 which could be obtained by sampling from  $\ell_i(\Gamma X)$ . This suggests that a 295

sketch which is constructed by drawing samples from  $\ell_i(X)$  is not too different compared to sampling from  $\ell_i(\Gamma X)$ . This intuition is supported by the following result which describes the change in the leverage scores after re-weighting a single row.

Proposition 3.7 ([24] Lemma 5). Let  $\Gamma^{\langle i \rangle} \in \mathbb{R}^{kd \times kd}$  be a diagonal matrix with  $\Gamma_{ii}^{\langle i \rangle} = \sqrt{\gamma} \in (0, 1)$  and  $\Gamma_{jj}^{\langle i \rangle} = 1$  for each  $j \neq i$ . Then

$$\ell_i(\Gamma^{\langle i \rangle} X) = \frac{\gamma \ell_i(X)}{1 - (1 - \gamma)\ell_i(X)} \le \ell_i(X)$$
(34)

302 and for  $i \neq j$ 

$$\ell_j(\Gamma^{\langle i \rangle} X) = \ell_j(X) + \frac{(1-\gamma)\ell_{ij}^2(X)}{1-(1-\gamma)\ell_i(X)} \ge \ell_j(X)$$
(35)

where  $\ell_{ij}(X) = (U_X U_X^T)_{ij}$  are the cross leverage scores.

Since  $U_X$  has orthogonal columns, we have  $||v|| = ||U_X v||$  for any  $v \in \mathbb{R}^{\rho}$ and thus the cross leverage scores from the above Lemma satisfy

$$\ell_i(X) = \sum_{j=1}^{kd} \ell_{ij}^2(X).$$
(36)

For a general diagonal matrix  $\Gamma$  as in Proposition 3.6 we may without loss of generality assume that each entry lies in (0, 1] since we can divide the elements by their maximum. The re-weighting can thus be considered as a superposition of single row operations

$$\Gamma = \prod_{i=1}^{kd} \Gamma^{\langle i \rangle} \tag{37}$$

where the  $\Gamma^{\langle i \rangle}$  are as in Proposition 3.7. Since the  $\Gamma^{\langle i \rangle}$  commute we can apply them in any order without changing the outcome. Considering Lemma 3.5, if we could ensure that  $\ell_i(X)$  isn't substantially smaller than  $\ell_i(\Gamma X)$  then sampling from  $q_i = \rho^{-1}\ell_i(X)$  will produce good sketches for  $\Gamma X$ .

Large leverage scores  $\ell_i(X) \approx 1$ . Equation (34) shows that the relative change of the *i*-th leverage score after a re-weighting of the *i*-th row shrinks when  $\ell_i(X) \to 1$ . In the extreme case when  $\ell_i(X) = 1$  the re-weighting has no effect. In addition to this stability property it trivially holds that  $\ell_i(X) \leq 1$  which suggests that large leverage scores are fairly stable when rows are re-weighted. Small leverage scores  $\ell_i(X) \ll 1$ . From Equation (35) we know that the increase of  $\ell_j(X)$  after re-weighting of row *i* is proportional to  $\ell_{ij}(X)$ . If the entries of the scaling matrix  $\Gamma$  don't vary too much, then (36) suggests that we can expect the total increase, i.e. after applying  $\Gamma^{\langle j \rangle}$  for each  $j \neq i$  to be roughly of order  $\ell_i(X) - \ell_i^2(X) \approx \ell_i(X)$ . On the other hand, small  $\ell_i(X)$  are fairly sensitive to re-weighting of row *i* since  $\ell_i(\Gamma^{\langle i \rangle}X) \approx (\Gamma_{ii}^{\langle i \rangle})^2 \ell_i(X)$  in that case. Thus we can expect that the re-weighting of row *i* will counterbalance the effects from re-weighting the other rows. In addition, we know that

$$\sum_{i=1}^{kd} \ell_i(X) = \sum_{i=1}^{kd} \ell_i(\Gamma X).$$

Since large leverage scores will likely be quite stable and  $\ell_i(\Gamma X) \geq 0$  we would expect that not too many small leverage scores will become large.

So far we have discussed the projection of the high-dimensional system 322 without providing explicit details on how the basis  $\Psi$  is selected. A desired 323 property is to sustain a small projection error for all admissible parameter 324 choices under the constraint  $\rho \ll n$ . Suitable options include subsets of 325 the right singular vectors of A or orthogonalised Krylov-subspace bases [25], 326 however these have to be computed for each individual parameter vector 327 which can be detrimental to the speed of the solver. Alternatively, we opt 328 for a generic basis exploiting the smoothness of u on domains with smooth 329 Lipschitz boundaries. A simple choice is to select the basis among the eigen-330 vectors of the discrete Laplacian operator 331

$$\Delta \doteq D^T Z_\Delta^2 D,\tag{38}$$

for  $Z_{\Delta}^2 = \text{diag}([|\Omega_1|, \ldots, |\Omega_k|] \otimes 1_d)$ . From  $U_{\Delta}^T \Delta U_{\Delta} = \Sigma_{\Delta}$  and splitting the eigenvectors as

$$U_{\Delta} = \left( U_{\Delta}^{(1:n-\rho-1)} | \Psi \right),$$

such that the columns of  $\Psi$  correspond to the last  $\rho$  columns of  $U_{\Delta}$ , and respectively to the  $\rho$  smallest eigenvalues  $\{\lambda_{n-\rho-1}(\Delta), \ldots, \lambda_n(\Delta)\}$ . In effect, with  $\Delta$  constrained by the Dirichlet boundary conditions, the norm  $\|\Delta\Psi^{(i)}\|$ provides a measure of the smoothness of  $\Psi^{(i)}$  in the interior of  $\Omega$ . It is not difficult to see that this basis satisfies

$$\|\Delta \Psi^{(i)}\| \ge \|\Delta \Psi^{(j)}\| \quad \text{for} \quad \rho \ge i > j \ge 1.$$

We remark that the computation of the basis is computationally very ex-332 pensive for large n, as the eigen-decomposition of  $\Delta$  is necessary, however 333 this is only computed once, prior to the beginning of the simulation (offline 334 stage) in an offline stage. After the matrix  $\Psi$  has been obtained we can com-335 pute the leverage scores  $\ell_i(Z_{\Delta}D\Psi)$ . The Laplacian  $\Delta$  differs from a general 336 stiffness matrix A only by different diagonal weights, i.e.  $Z^2_{\Delta}$  is replaced by 337 the diagonal matrix  $Z^2 = Z^2_{\Delta} \operatorname{diag}[(p_1, \ldots, p_k) \otimes 1_d]$  where the  $p_i$  contain 338 information about the parameter from (1). Propositions 3.6 and 3.7 along 339 with the developments thereafter suggest that the Laplacian leverage scores 340  $\ell_i(Z_{\Delta}D\Psi)$  can nonetheless be used to construct sketches  $\hat{G} = X^T \tilde{S} S^T X$  of 341 the projected matrix  $G = X^T X = \Psi^T Y^T Y \Psi$  because the difference in the 342 stiffness matrices is just a diagonal weighting. 343

#### 344 4. Complexity and error analysis

Motivated by the developments from the previous sections we propose the following algorithm for computing solutions to a sequence of N problem of the form (1). We assume that each problem is specified by its parameter vector  $z^{(t)} \in \mathbb{R}^{kd}$  for  $t = 1, \ldots, N$  (see section 2.1).

The complexity and approximation error of Algorithm 1 are obviously linked. The more samples we draw the better we expect our solutions to be. Although the size of the reduced system matrix G (and therefore its sketched counterpart  $\hat{G}$  as well) is independent of c, the computational burden for building  $\hat{G}$  is higher when drawing more samples. More precisely, we need:

- $\mathcal{O}(c)$  operations in order to find  $\mathbf{i}_1, \dots \mathbf{i}_c \stackrel{\text{iid}}{\sim} q$ . This is possible because q is fixed and we can perform the necessary pre-processing offline [26].
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•  $\mathcal{O}(c)$  operations for computing the sampled indices  $\{\mathbf{j}_1, \ldots, \mathbf{j}_{c'}\}$  and their frequencies  $m_j$  as this requires a single loop through the set  $\{\mathbf{i}_1, \ldots, \mathbf{i}_c\}$  of initial samples.

- $\mathcal{O}(c')$  operation for assembling the diagonal matrices M and  $\hat{Z}$ .
- $\mathcal{O}(c'\rho)$  operations for computing  $M\hat{Z}D_{(J)}\Psi$ . This can be achieved since computing  $M\hat{Z}D_{(J)}$  requires  $\operatorname{nnz}(D_{(J)}) = \mathcal{O}(c')$  multiplications and  $\rho \cdot \operatorname{nnz}(M\hat{Z}D_{(J)}) = \rho \cdot \operatorname{nnz}(D_{(J)}) = \mathcal{O}(\rho c')$  multiplications are enough for computing  $[M\hat{Z}D_{(J)}]\Psi$  due to sparsity of D.

input : Matrices  $D \in \mathbb{R}^{kd \times n}$ ,  $\Psi \in \mathbb{R}^{n \times \rho}$ , data vector  $\Psi^T b \in \mathbb{R}^{\rho}$ , and sampling probabilities  $q_i = \rho^{-1} \ell_i(Z_\Delta D \Psi)$  (offline)

**output:** Parameter dependent solutions  $\hat{r}^{(t)} \in \mathbb{R}^{\rho}$  where t = 1, ..., NOnline Simulation;

for  $t \leftarrow 1$  to N do

**input** : Parameter vector  $z^{(t)} \in \mathbb{R}^k$ , sample size cdraw row indices  $\mathbf{i}_1, \dots, \mathbf{i}_c \stackrel{\text{id}}{\sim} q$  from [kd]; get the sampled indices  $J = \bigcup_{j=1}^c {\{\mathbf{i}_j\}}$ ; set c' = |J| and write  $J = {\{\mathbf{j}_1, \dots, \mathbf{j}_{c'}\}}$ ; compute the frequencies  $m_j = \sum_{k=1}^c \delta(\mathbf{i}_k = \mathbf{j}_j)$  for  $j = 1, \dots, c'$ ; find  $M_{jj}^2 = c^{-1}m_j q_{\mathbf{j}_j}^{-1}$  for  $j = 1, \dots, c'$  and the diagonal matrix M; find  $\hat{Z}_{jj}^2 = z_{\mathbf{j}_j}^{(t)}$  for  $j = 1, \dots, c'$  and the diagonal matrix  $\hat{Z}^2$ ; assemble the  $c' \times \rho$  matrix  $\hat{X} = M\hat{Z}D_{(J)}\Psi$ ; compute reduced system  $\hat{G} = \hat{X}^T\hat{X}$ ; compute and store  $\hat{r}^{(t)} \leftarrow \text{solve}(\hat{G}, \Psi^T b)$ ;



Algorithm 1: Algorithm for simulating the low-dimensional projected solution of the FEM equations for different choices of parameter vectors p. Note that as we are sampling with replacement,  $c' \leq c$ . In the above  $\delta(\cdot)$ denotes the indicator function where  $\delta(E) = 1$  if the event E has occurred and it is zero otherwise otherwise.  $D_{(J)}$  is the sub-matrix of D whose rows are the (ordered) elements of J

•  $\mathcal{O}(c'\rho^2)$  operations in order to build  $\hat{G}$  which corresponds to the cost of multiplication for dense matrices.

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•  $\mathcal{O}(\rho^3)$  operations for solving  $\hat{G}r = \Psi^T b$  with a direct method.

The sketch  $\hat{G}$  will be singular if we draw  $c' < \rho$  distinct samples which 367 means that building the sketch  $\hat{G}$  dominates the complexity of Algorithm 368 1. In particular, the worst case complexity doesn't exceed  $\mathcal{O}(c\rho^2)$  since we 369 require  $c \ge c' \ge \rho$ . If the sampling probabilities are a good approximation 370 in the sense that  $\beta$  in Lemma 3.5 can be chosen close to 1, then we need 371  $c = \mathcal{O}(\varepsilon^{-2}\rho\log(\rho))$  samples in order to have a provably controlled error. The 372 worst case, i.e. the the largest increase of  $\ell_i(X)$ , will be observed if  $z_i^{(t)} \ll z_i^{(t)}$ 373 for  $j \neq i$ . A parameter p corresponding to such a situation essentially renders 374

the implementation of the classical Galerkin FEM problematic, as  $\kappa(A)$  scales to  $p_{\text{max}}/p_{\text{min}}$ , see Theorem 5.2 in [19] The following theorem summarises the findings of this section.

**Theorem 4.1.** Let  $\varepsilon \in (0, 1)$  and  $\beta \in (0, 1]$  is such that the sampling probabilities  $q_i$  from Algorithm 1 satisfy (31), i.e.

$$q_i \ge \beta \frac{\ell_i(ZD\Psi)}{\rho} \quad i = 1, \dots, kd$$

where  $Z^2 = \operatorname{diag}(z^{(t)})$ . Let  $G = X^T X = \Psi^T D^T Z^2 D \Psi$  be the reduced system matrix corresponding to parameter  $z^{(t)}$  and  $\kappa(G)$  its condition number. For the choice  $c = 15\rho \log(15\rho)\beta^{-1}\varepsilon^{-2}$  Algorithm 1 requires  $\mathcal{O}(\rho^3 \log(\rho)\beta^{-1}\varepsilon^{-2})$ operations and outputs, with probability exceeding 0.999, a vector  $\hat{r}^{(t)}$  that satisfies

$$\frac{\|\hat{r}^{(t)} - G^{-1}\Psi^T b\|}{\|G^{-1}\Psi^T b\|} \le \sqrt{\kappa(G)} \frac{\varepsilon}{1-\varepsilon}.$$
(39)

*Proof.* As stated before, the complexity of Algorithm 1 is  $\mathcal{O}(c\rho^2)$  which immediately implies that it requires  $\mathcal{O}(\rho^3 \log(\rho)\beta^{-1}\varepsilon^{-2})$  operations for a single query. It remains to prove the error bound. In view of (29) and the developments thereafter it follows, conditional on  $\hat{G}$  being invertible, that

$$\frac{\|\hat{r}^{(t)} - G^{-1}\Psi^{T}b\|}{\|G^{-1}\Psi^{T}b\|} \leq \|\Sigma_{X}^{-1}(U_{X}^{T}SS^{T}U_{X})^{-1}\Sigma_{X} - I\|$$
$$\leq \kappa(X)\|(U_{X}^{T}SS^{T}U_{X})^{-1} - I\|$$
$$\leq \kappa(X)\frac{1}{1-\varepsilon}\|U_{X}^{T}SS^{T}U_{X} - I\|.$$

Since  $\kappa^2(X) = \kappa(G)$  we only need to show that

$$\mathbb{P}(\|U_X^T S S^T U_X - I\| \ge \varepsilon) \le 0.001$$

because  $\hat{G}$  is necessarily invertible on that event which implies validity of the estimates from before. But plugging the value for c into (32) we obtain for any  $\rho \geq 1$ 

$$\mathbb{P}(\|U_X^T S S^T U_X - I\| \ge \varepsilon) \le \frac{2}{15} \exp\left(-\frac{29}{16}\log(15\rho)\right) < 0.001.$$

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Algorithm 1 is most attractive when we can tolerate an error somewhere between 1% to 10% in which case we can obtain the solution to a single query in about  $\mathcal{O}(\beta^{-1}\rho^3 \log(\rho))$  time. In practice the value for  $\beta$  is unobtainable since it requires knowledge of the true leverage scores but considering Lemma 3.7 and the arguments thereafter, we expect that for a moderately large  $\beta^{-1}$ the required bound will hold for all but a few small leverage scores. The statement in Lemma 3.5 is rather pessimistic when there are few misaligned leverage scores since it requires a uniform bound. For practical purposes we expect that  $\beta^{-1}$  can be substituted with a small constant and we take  $\varepsilon = 0.1$  which will ensure reglarity of the sketch. Up until now we have only considered the randomisation error of the sketched solution, i.e. we have analysed  $\|\hat{u}_{\text{reg}} - u_{\text{reg}}\|$ . However, the the total error of  $\hat{u}_{\text{reg}}$  compared to the high dimensional solution u of (7) has two components. If we decompose the process into two steps

$$\min_{u \in \mathbb{R}^n} \|Yu - (Y^T)^{\dagger}b\|^2 \quad \xrightarrow{\text{Projection}} \quad \min_{u \in \mathcal{S}_{\rho}} \|Yu - (Y^T)^{\dagger}b\|^2 \tag{40}$$

$$\min_{u\in\mathcal{S}_{\rho}}\|Yu-(Y^T)^{\dagger}b\|^2 \quad \xrightarrow{\text{Sketching}} \quad \min_{u\in\mathcal{S}_{\rho}}\|\hat{Y}\Pi u-(\Psi^T\hat{Y}^T)^{\dagger}\Psi^Tb\|^2, \quad (41)$$

it becomes apparent that even with a perfect sketch, i.e. if we solved the noiseless projected problem (15) and (41) is negligible, we could still not achieve an error smaller than  $||u_{opt} - \Pi u_{opt}||$ . The next result tells us that the error from (40) is close to the optimal one.

**Theorem 4.2.** Let  $u_{\text{opt}}$  be the solution of (7) and  $u_{\text{reg}}$  be the optimum of (15). If  $\kappa(A)$  is the condition number of the stiffness matrix A and  $\Pi = \Psi \Psi^T$  the projection ont  $S_{\rho}$ , then

$$\|u_{\text{opt}} - u_{\text{reg}}\| \le \left(1 + \sqrt{\kappa(A)}\right) \|u_{\text{opt}} - \Pi u_{\text{opt}}\|.$$

*Proof.* Recall that  $A = Y^T Y$  and  $G = X^T X = \Psi^T Y^T Y \Psi$ . From the developments in Lemma 3.2 we know that  $u_{\text{reg}} = \Psi G^{-1} \Psi^T b$ . We may write as before  $X = U_X \Sigma_X V_X^T$  so that  $G^{-1} = V_X \Sigma_X^{-2} V_X^T$  and

$$\begin{aligned} \|u_{\text{opt}} - u_{\text{reg}}\| &= \|u_{\text{opt}} - \Psi G^{-1} \Psi^T b\| \\ &= \|u_{\text{opt}} - \Psi G^{-1} \Psi^T A u_{\text{opt}}\| \\ &= \|u_{\text{opt}} - \Psi G^{-1} \Psi^T A [\Pi + (I - \Pi)] u_{\text{opt}}\| \\ &\leq \|u_{\text{opt}} - \Psi G^{-1} \Psi^T A \Psi \Psi^T u_{\text{opt}}\| + \|\Psi G^{-1} \Psi^T A (I - \Pi) u_{\text{opt}}\| \end{aligned}$$

where the last line follows from the triangle inequality and the fact that  $\Pi = \Psi \Psi^T$ . Since  $\Psi^T A \Psi = \Psi^T Y^T Y \Psi = X^T X = G$  the expression in the first term of the above equation simplifies to

$$u_{\rm opt} - \Psi G^{-1} (\Psi^T A \Psi) \Psi^T u_{\rm opt} = u_{\rm opt} - \Pi u_{\rm opt}.$$

In order to simply the second term we can start by writing

$$\Psi^T A = \Psi^T Y^T Y = X^T Y = (U_X \Sigma_X V_X^T)^T Y = V_X \Sigma_X U_X^T Y$$

which implies that

$$G^{-1}\Psi^T A = V_X \Sigma_X^{-2} V_X^T V_X \Sigma_X U_X^T Y = V_X \Sigma_X^{-1} U_X^T Y.$$

From those observation it follows that

$$\begin{aligned} \|u_{\text{opt}} - u_{\text{reg}}\| &\leq \|u_{\text{opt}} - \Pi u_{\text{opt}}\| + \|\Psi V_X \Sigma_X^{-1} U_X^T Y (I - \Pi) u_{\text{opt}}\| \\ &\leq \|u_{\text{opt}} - \Pi u_{\text{opt}}\| \left(1 + \|\Psi V_X \Sigma_X^{-1} U_X^T Y\|\right). \end{aligned}$$

If we write  $\lambda_{\min}(A)$  and  $\lambda_{\max}(A)$  for the smallest and largest eigenvalues of A, then it must hold that

$$\lambda_{\min}(A) \le \lambda_{\min}(G) \le \lambda_{\max}(G) \le \lambda_{\max}(A)$$

because  $\Psi$  has orthogonal columns. Indeed, if  $\mathbb{S}^{n-1} \doteq \{w \in \mathbb{R}^n : ||w|| = 1\}$  is the *n*-dimensional unit sphere, then

$$\min_{w \in \mathbb{S}^{n-1}} w^T A w \le \min_{w \in \mathcal{S}_{\rho} \cap \mathbb{S}^{n-1}} w^T A w \le \max_{w \in \mathcal{S}_{\rho} \cap \mathbb{S}^{n-1}} w^T A w \le \max_{w \in \mathbb{S}^{n-1}} w^T A w$$

is obviously true. Since the columns of  $\Psi$  form an ONB of  $\mathcal{S}_\rho$  we have

$$\min_{w \in S_{\rho} \cap \mathbb{S}^{n-1}} w^T A w = \min_{w \in \mathbb{S}^{\rho-1}} w^T \Psi^T A \Psi w = \min_{w \in \mathbb{S}^{\rho-1}} w^T G w = \lambda_{\min}(G)$$
$$\max_{w \in S_{\rho} \cap \mathbb{S}^{n-1}} w^T A w = \max_{w \in \mathbb{S}^{\rho-1}} w^T \Psi^T A \Psi w = \max_{w \in \mathbb{S}^{\rho-1}} w^T G w = \lambda_{\max}(G).$$

Thus,  $\|\Sigma_X^{-1}\|^2 = \lambda_{\min}^{-1}(G) \leq \lambda_{\min}^{-1}(A)$ . Clearly we also have  $\|Y\|^2 = \lambda_{\max}(A)$ . Due to orthogonality we know that  $\|\Psi\| = \|V_X\| = \|U_X\| = 1$ . Combining those estimates we obtain

$$\|\Psi V_X \Sigma_X^{-1} U_X^T Y\| \le \sqrt{\frac{\lambda_{\max}(A)}{\lambda_{\min}(G)}} \le \sqrt{\kappa(A)},$$

<sup>388</sup> which yields the desired bound.

- 1		a.

If the subspace  $S_{\rho}$  is such that the relative projection error is small, then the norm of  $u_{\text{reg}}$  will be similar to the norm of  $u_{\text{opt}}$ . More precisely,

$$\frac{\|u_{\text{reg}} - u_{\text{opt}}\|}{\|u_{\text{opt}}\|} \le \delta \implies \frac{\|u_{\text{reg}}\|}{\|u_{\text{opt}}\|} \in [1 - \delta, 1 + \delta]$$

so that Theorem 4.1 applies to  $||u_{reg} - \hat{u}_{reg}|| / ||u_{opt}||$  with a small  $\delta$ -dependent constant. By combining the previous two theorems we obtain the following.

**Corollary 4.3.** Let  $\varepsilon_{\rm R} \in (0,1)$  and assume that the assumptions of Theorem 4.1 are satisfied for  $\varepsilon = \varepsilon_{\rm R}$ . If  $u_{\rm opt}$  is the solution of (7) and the subspace  $S_{\rho}$  is such that

$$\|u_{\text{opt}} - \Pi u_{\text{opt}}\| \le \|u_{\text{opt}}\|\varepsilon_{\mathrm{P}}\|$$

for some  $\varepsilon_{\rm P} \in (0,1)$ . Then the total error of the solutions  $\hat{u}_{\rm reg} = \Psi \hat{r}$  produced by Algorithm 1 satisfy the bound

$$\frac{\|u_{\rm opt} - \hat{u}_{\rm reg}\|}{\|u_{\rm opt}\|} \le \left(1 + \varepsilon_{\rm P}\sqrt{\kappa(A)}\right)\sqrt{\kappa(G)}\frac{\varepsilon_{\rm R}}{1 - \varepsilon_{\rm R}} + \left(1 + \sqrt{\kappa(A)}\right)\varepsilon_{\rm P}.$$
 (42)

*Proof.* We can start with the estimate

$$\frac{\|u_{\rm opt} - \hat{u}_{\rm reg}\|}{\|u_{\rm opt}\|} \le \frac{\|u_{\rm opt} - u_{\rm reg}\|}{\|u_{\rm opt}\|} + \frac{\|u_{\rm reg} - \hat{u}_{\rm reg}\|}{\|u_{\rm opt}\|}$$

Using the estimate from Theorem 4.2 we get

$$\frac{\|u_{\rm opt} - u_{\rm reg}\|}{\|u_{\rm opt}\|} \le \left(1 + \sqrt{\kappa(A)}\right) \frac{\|u_{\rm opt} - \Pi u_{\rm opt}\|}{\|u_{\rm opt}\|} \le \left(1 + \sqrt{\kappa(A)}\right) \varepsilon_{\rm P}.$$

It remains to bound the other term. Since  $\Psi$  has orthogonal columns we obtain from Theorem 4.1

$$\frac{\|u_{\rm reg} - \hat{u}_{\rm reg}\|}{\|u_{\rm reg}\|} \le \sqrt{\kappa(G)} \frac{\varepsilon_{\rm R}}{1 - \varepsilon_{\rm R}} \implies \frac{\|u_{\rm reg} - \hat{u}_{\rm reg}\|}{\|u_{\rm opt}\|} \le \frac{\|u_{\rm reg}\|}{\|u_{\rm opt}\|} \sqrt{\kappa(G)} \frac{\varepsilon_{\rm R}}{1 - \varepsilon_{\rm R}}.$$

Since we have shown in the proof of Theorem 4.2 that

$$u_{\rm reg} = \Pi u_{\rm opt} + \Psi G^{-1} \Psi^T A (I - \Pi) u_{\rm opt}$$

we can estimate

$$||u_{\rm reg}|| \le ||\Pi u_{\rm opt}|| + ||\Psi G^{-1} \Psi^T A (I - \Pi) u_{\rm opt}|| \le ||u_{\rm opt}|| + \sqrt{\kappa(A)} ||(I - \Pi) u_{\rm opt}||.$$

As before, we have used the fact that

$$\Psi G^{-1} \Psi^T A = \Psi V_X \Sigma_X^{-1} U_X^T Y \implies \|\Psi G^{-1} \Psi^T A\| \le \sqrt{\kappa(A)}.$$

From  $||u_{\text{opt}} - \Pi u_{\text{opt}}|| \le \varepsilon_{\text{P}} ||u_{\text{opt}}||$  it follows that

$$\frac{\|u_{\rm reg}\|}{\|u_{\rm opt}\|} \le 1 + \varepsilon_{\rm P} \sqrt{\kappa(A)},$$

<sup>393</sup> which completes the proof.

If we assume that  $\varepsilon_{\rm P}\sqrt{\kappa(G)} \approx 1$ , then the error estimate from Corollary 4.3 states, with small leading constants, that

$$\frac{\|u_{\text{opt}} - \hat{u}_{\text{reg}}\|}{\|u_{\text{opt}}\|} \le \mathcal{O}\left((\varepsilon_{\text{R}} + \varepsilon_{\text{P}})\sqrt{\kappa(A)}\right).$$

It therefore makes sense to have a sketching error  $\varepsilon_{\rm R}$  that is of the same order 394 as the projection error  $\varepsilon_{\rm P}$ . In practice we found that projection errors of 395 roughly 1% to 10% can be expected so that the sketching induced error isn't 396 very harmful if we choose the sample size as in Theorem 4.1 with  $\varepsilon_{\rm R} = 0.1$ . 397 As illustrated in (40) and (41), the accuracy in our approach is limited by 398 both, the subspace projection and sketching error. The proposed method 399 is therefore most useful when a moderate error of 1%-10% is acceptable in 400 each query. In situations where the solutions of the FEM system are used 401 for further computations that require substantially more accurate solutions 402 it would be necessary to select a large number of basis elements and thus 403 a large number of samples as well. This makes the queries computationally 404 more expensive and the approach much less appealing. 405

#### 406 5. Numerical results

To test the performance of Algorithm 1 we consider the finite element formulation of the elliptic equation (1) with homogeneous Dirichlet boundary conditions u = 0 on  $\partial \Omega$  and a forcing term derived from a piecewise constant approximation of the function

$$f(x) = \begin{cases} 5 & \text{if } \sqrt{(x_1 + \frac{1}{2})^2 + x_2^2 + x_3^2} \le 0.3, \\ 0 & \text{otherwise,} \end{cases}$$

We discretise the model on a spherical domain  $\Omega$  (d = 3) of unit radius 407 comprising k = 684560 unstructured linear tetrahedral elements. This leads 408 to a total 116805 nodes of which n = 101509 are situated in the interior of 409 the domain. In these circumstances X is a tall matrix with 2053680 rows, 410 the stiffness matrix A has dimensions  $101509 \times 101509$  and the sample space 411 is [2053680]. To test how out sketching algorithm performs in increasing 412 problem dimensions, we run some tests on a finer discretisation of the domain 413 with k = 1688869 elements and 315744 with n = 257374 are in the interior, 414 vielding sample space of dimension 5066607. Given that the corresponding 415 results are very similar and result in the same conclusions we haven't included 416 those in full detail. 417

We seek to assess the practical performance of our algorithm in terms 418 of its speed and accuracy in computing the sketched solution under various 419 choices sampling budgets and low-dimensional subspaces, for the proposed 420 sampling distribution. To achieve this we perform three benchmark tests 421 involving realisations of (i) a uniformly distributed random parameter field, 422 (ii) a smoothly varying lognormal random field, and (iii) a random field with 423 jump discontinuities. For each of these we run a sequence of N = 100 simu-424 lations, i.e. p queries, and record timings and error measures on average. For 425 each realisation we compute also the conventional FEM solution to provide 426 a reference for comparison. The high-dimensional  $u_{opt}$  is computed using 427 Matlab's built-in A b command [27]. Given that this is not very efficient 428 and thus not the best performance benchmark we have additionally provided 429 times corresponding to the computation of an approximate, i.e. stopped at 430 10% error tolerance, solution  $u_{\rm PCG}$  using a preconditioned conjugate gradient 431 (PCG) method. Our code was implemented in Matlab R2018b and executed 432 on a workstation equipped with two 14-core Intel Xeon dual processors, run-433 ning Linux NixOS with 384GB RAM. 434

In the offline phase of Algorithm 1 we form a low-dimensional ONB for 435 the projection by computing the last eigenfunctions of the sparse Laplacian 436 matrix discretised on  $\Omega$ . For this time consuming and memory demanding 437 operation we have resorted to the **svds** and **qr** commands which avoid com-438 puting the complete spectrum or they produce a sparse ONB respectively. 430 The computation of the sampling distribution based on the leverage scores 440 of  $X_{\Delta} = Z_{\Delta}D\Psi$  was also performed once during the offline phase and took 441 about 4 hours, using the svd(, econ') command. The distribution q was 442 sampled with replacement during the online phase of the algorithm using 443 uniformly random numbers in combination with histc (which performs a 444

binary search on the cumulative probabilities), which indicatively, for the chosen q, outputs a million samples in about 0.3 s. Notice that although this sampling implementation is not independent of the dimension kd, there exist alternative schemes that can handle arbitrarily large distributions with constant complexity [26].

In the implementation of the algorithm we record the following quantities-450 diagnostics that provide evidence on the performance in the conditions of 451 each benchmark: the ratio c'/3k indicating how many of the rows of X are 452 used in the sketch, the relative subspace projection error  $\|\Pi u_{opt} - u_{opt}\| / \|u_{opt}\|$ , 453 the upper bound of the randomisation error  $\|\hat{G}^{-1}G - I\|$ , the relative regres-454 sion error  $\|\hat{u}_{\text{reg}} - u_{\text{reg}}\| / \|u_{\text{reg}}\|$ , and the relative total error  $\|\hat{u}_{\text{reg}} - u_{\text{opt}}\| / \|u_{\text{opt}}\|$ . 455 In the context of real-time model prediction in manufacturing processes an 456 upper limit of 10% for the total error is deemed reasonable. 457

#### 458 5.1. Uniformly random parameter field

In this first instance we simulate sketched solutions for 100 parameter vectors  $p \in \mathbb{R}^k$  drawn at random from  $\mathcal{U}([10^{-1}, 10^2])$ . Five sets of simulations were performed using ONBs incorporating the last  $\rho = \{50, 100\}$  singular functions of the Laplacian. Our focus was on monitoring the trade-off between accuracy and time consumption when  $c = \{5 \times 10^5, 10^6, 5 \times 10^6\}$  iid samples are drawn from p. The results are tabulated in table 1.

Although the values in p vary over four orders of magnitude, the param-465 eter has a homogeneous expectation within the domain and thus overall the 466 algorithm yields sketched solutions at 10% or less total error, with only 100 467 basis functions. The results show that the sampling is highly non-uniform 468 since even in the case where a million idd samples were taken these involved 469 only 41074, a mere 6%, of the rows of X. The sketching-induced error factor 470  $\|\hat{G}^{-1}G - I\|$  appears to reduce almost linearly with the number of sam-471 ples c. Comparing the relative subspace projection  $\|\Pi u_{opt} - u_{opt}\|$  and total 472  $\|\hat{u}_{\rm reg} - u_{\rm opt}\|$  errors note that for  $\|\hat{G}^{-1}G - I\| \approx 1$  the later is kept marginally 473 larger than the former, which verifies the regularising effect of the projection 474 on the sketching-induced noise. It is also important to see that in switching 475 from  $\rho = 50$  to  $\rho = 100$  the projection error is halved to 0.03, however the 476 number of samples necessary to yield the same levels of the error increases by 477 about 5 times. For relative error tolerances around the 10% mark, the times 478 recorded for the smaller mesh are about 0.5 s, while by comparison the time 479 for computing a solution  $u_{PCG}$  using a preconditioned conjugate gradient 480 solver (up to the same 10% error tolerance) took 2.40 s (on average from 100 481

ρ	$c \ [10^6]$	time [s]	c'/3k	$\frac{\ \Pi u_{\rm opt} - u_{\rm opt}\ }{\ u_{\rm opt}\ }$	$\ \hat{G}^{-1}G - I\ $	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{reg}}\ }{\ u_{\mathrm{reg}}\ }$	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{opt}}\ }{\ u_{\mathrm{opt}}\ }$
50	0.5	0.25	0.04	0.07	1.60	0.07	0.09
50	1	0.46	0.06	0.07	1.07	0.05	0.08
100	0.5	0.34	0.04	0.03	3.99	0.11	0.11
100	1	0.52	0.06	0.03	2.30	0.06	0.07
100	5	2.36	0.11	0.03	0.77	0.02	0.04

Table 1: Numerical results for the tests performed with  $p \sim \mathcal{U}([10^{-1}, 10^2])$ . The quantities above are averages over 100 runs with different p realisations. The results show the impact of c and  $\rho$  on the various error components and the computing times. Note that for a sufficiently large c the total error is only marginally larger than the projection error, which manifest the regularising effect of the projection on the sketching induced error.

<sup>482</sup> runs) on the smaller mesh (n = 101509). Computing a PCG solution on the <sup>483</sup> larger grid (n = 257374) took on average 3.46 s with relative improvements <sup>484</sup> similar to those on the smaller mesh for a 10% error tolerance.

The trade-off between speed and accuracy can be seen by comparing the 485 results in the first and last rows of the table 1 where the algorithm achieves a 486 4% total error, when the projection error is at 3%, after five million samples. 487 On the other hand, solutions within a 10% error margin, when the projection 488 error is at 7%, are obtained in less than 0.5 s, which is about 5 times faster 489 than computing a comparable PCG solution. The histograms in figure 1 490 provide a further insight on how the various error components vary within 491 the ensemble of the 100 problems. We point out that the numerical results 492 are in good agreement with the assertion of Theorem 4.1. For the example 493 shown in figure 1, i.e. when  $\rho = 50$  and the error tolerance is  $\varepsilon = 10\%$ , 494 our theorem predicts  $c = 15\rho \log(15\rho)\beta^{-1}\varepsilon^{-2} \approx 5.0 \cdot 10^5\beta^{-1}$  samples which is 495 consistent to the observed c = 1 when  $\beta^{-1} \approx 2$ . In the histograms we see that 496 the sketching error virtually never exceeds 10% and that  $\|\hat{G}^{-1}G - I\|$  exhibits 497 the same pattern as  $||u_{\text{opt}} - u_{\text{reg}}|| / ||u_{\text{opt}}||$  which supports the claim that this 498 quantity is driving the sketching error. Similar observations can be made for 499 the other cases of table 1. Figure 1 also shows that, although their magnitude 500 is comparable, the variability in the projection error is much smaller than 501 that of the sketching error. This is not surprising as the sketching is an 502 intrinsically random method while the differences in the projection are only 503 due to perturbations in the parameter. 504



Figure 1: Histograms showing the variation in the various error quantities relating to the performance of our algorithm, as recorded in the table 1 for 100 different realisations of the p vector from  $\mathcal{U}([10^{-1}, 10^2])$  of the code with  $\rho = 50$  and c = 1 million.

#### 505 5.2. Smooth parameter field

In the second benchmark we turn our attention to parameter functions with smooth spatial variation like those encountered in the context of uncertainty quantification for PDEs [6]. As the anticipated FEM solution is smooth we maintain the bases used in 5.1. In this case, the parameter p is a lognormal random field given by  $p \doteq \exp(b)$ , where b is a zero-mean Gaussian random field with Whittle-Matérn covariance function with smoothness parameter  $\nu > 0$  given by

$$C_b(x,y) = \frac{\operatorname{Var}[b]}{2^{\nu-1}\Gamma(\nu)} \left( \|x-y\|_M \right)^{\nu} K_{\nu} \left( \|x-y\|_M \right), \quad x,y \in \Omega,$$
(43)

where  $\Gamma(\nu)$  is the Gamma function,  $||x||_M^2 = x^T M^{-1} x$  is the weighted Euclidean norm with positive definite matrix M and  $K_{\nu}$  is the order  $\nu > 0$ modified Bessel function of the second kind. Here we use  $\nu = 15/2$ ,  $M^{1/2} =$ diag(1/5, 1/5, 1/5) and Var[b] = 1. We draw realisations of p by calculating once the Karhunen-Loève expansion of b and then drawing iid from  $\mathcal{N}(0, 1)$ .

The results presented in table 2 show a similar performance to the uni-518 formly random case in subsection 5.1. The suitability of the low-dimensional 519 subspace is evidenced by the 7% relative projection error attained at  $\rho = 50$ . 520 Sketched solutions within an error tolerance of 10% were computed in less 521 than 1 s. The timings of the PCG solutions were similar to those correspond-522 ing to the uniformly random parameter fields from the previous section and 523 took approximately 5 times longer to compute. Further, note that the total 524 error is within a 2% margin from the projection error, which demonstrates 525 the effectiveness of our sketching regularisation approach, apart from the test 526 with  $\rho = 100$  and c = 1 where  $\|\hat{G}^{-1}G - I\|$  is considerably higher, implying 527 that c was insufficiently small for that test. This observation is consistent 528 with our error bound in (4.1). Comparing the results for ( $\rho = 50, c = 5$ ) 520 and  $(\rho = 100, c = 1)$  shows that in the former case, although using half the 530 number of basis functions and five times more samples, due to the larger 531 projection error, the total error is still 1% larger than that of the later. The 532 images presented in figure 2 correspond to one of the simulations in this 533 benchmark with  $\rho = 100$  and c = 1 million, illustrating a cross section of the 534 profile of p, the exact FEM solution, the sketched solution and the relative 535 error between the two. 536



Figure 2: At the top left (a), a view of a lognormal field p sampled from the Whittle-Mattérn class, and to its right (b) the corresponding view of  $u_{opt}$ . Below to the left (c), the sketched projected solution  $\hat{u}_{reg}$  and to its right (d) the profile of the relative error between  $u_{opt}$  and  $\hat{u}_{reg}$ . All illustrations correspond to cross-sections of 3-dimensional functions at z = 0.

ρ	$c \ [10^6]$	time [s]	c'/3k	$\left  \begin{array}{c} \frac{\ \Pi u_{\mathrm{opt}} - u_{\mathrm{opt}}\ }{\ u_{\mathrm{opt}}\ } \right $	$\ \hat{G}^{-1}G - I\ $	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{reg}}\ }{\ u_{\mathrm{reg}}\ }$	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{opt}}\ }{\ u_{\mathrm{opt}}\ }$
25	0.5	0.23	0.04	0.15	0.73	0.05	0.16
50	) 1	0.45	0.06	0.07	0.95	0.04	0.08
50	5	1.99	0.12	0.07	0.35	0.02	0.07
10	0 1	0.56	0.06	0.03	1.97	0.05	0.06
10	0 5	2.16	0.12	0.03	0.65	0.04	0.04

Table 2: Numerical results for the tests with lognormal random field drawn from a Whittle-Matérn model with a smooth covariance. The algorithm yields solutions with less than 10% error with as few as 50 basis functions. Similar to the uniformly random case in table 1, the total errors are sustained close to the projection errors when  $\|\hat{G}^{-1}G - I\| < 1$ .

#### 537 5.3. Non-smooth parameter field

A more challenging benchmark test is to consider the FEM solution for a parameter field with non-smooth variation. In this case it is natural to anticipate that any significant jump discontinuities in the profile of p will have an adverse effect on the condition number of the stiffness matrix [19]. For our simulations we choose a piecewise constant approximation of the positive function

$$p(x) \doteq 9.1 + \operatorname{sgn}(x_1) + 3\operatorname{sgn}(x_2) + 5\operatorname{sgn}(x_3) + 0.1\mathcal{U}([0,1])$$

which is discontinuous along the three axes. The sign function  $\operatorname{sgn} : \mathbb{R} \to \mathbb{R}$ is given by  $\operatorname{sgn}(x) = x/|x|$  when  $x \neq 0$  and  $\operatorname{sgn}(0) = 0$ . In constructing the projection subspace we found that the smooth basis utilised in the previous cases was not appropriate to this case and we thus resorted in a sparse ONB taking a subset of the columns of the sparse unitary matrix computed from the QR decomposition of the Laplacian.

The results in table 3 suggest that the chosen basis is not very appropriate 544 since not only the number of basis functions is substantially larger, but also 545 the reduction in the projection error for a 100% increase in  $\rho$  is quiet marginal. 546 In turn, this increase in the dimension of  $\hat{G}$  affects the level of sketching 547 error, as even with c = 5 million samples  $\|\hat{G}^{-1}G - I\| > 1$ . Consequently, 548 this has a profound effect on timings which are slightly worse than those 540 corresponding to a PCG approach. For the tests for  $(\rho = 2 \times 10^3, c = 10^6)$ 550 and  $(\rho = 2 \times 10^3, c = 5 \times 10^6)$  notice that increasing the samples by five 551 times does not yield a significant improvement in the results, which is likely 552 triggered by the large  $\kappa(A) \approx 10^5$  in the error term of Theorem 4.2 which 553 causes the  $||u_{\rm reg} - u_{\rm opt}||$  to grow. 554

ρ	$c \ [10^6]$	time [s]	c'/3k	$\frac{\ \Pi u_{\rm opt} - u_{\rm opt}\ }{\ u_{\rm opt}\ }$	$\ \hat{G}^{-1}G - I\ $	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{reg}}\ }{\ u_{\mathrm{reg}}\ }$	$\frac{\ \hat{u}_{\mathrm{reg}} - u_{\mathrm{opt}}\ }{\ u_{\mathrm{opt}}\ }$
1000	1	2.67	0.06	0.07	4.61	0.01	0.26
1000	5	5.96	0.12	0.05	1.25	0.01	0.26
2000	1	4.87	0.06	0.02	77.36	0.02	0.08
2000	5	9.95	0.12	0.03	9.64	0.01	0.08

Table 3: Numerical results for the non-smooth parameter field. In this case the algorithm requires a far more extensive basis, and thus considerably more samples and computing time to yield solutions within the required 10% error margin.

#### 555 6. Conclusions

We have considered expediting the solution of the finite element method 556 equations arising from the discretisation of elliptic PDEs on high-dimensional 557 models. Taking into consideration the multi-query context and the smooth 558 profile of the FEM solution, we proposed a practical sketch-based algorithm 559 that involves projection onto lower-dimensional subspace and sketching us-560 ing a generic, sampling distribution derived from the leverage scores of a tall 561 matrix associated with the Laplacian operator. We have elaborated on the 562 impact of the projection in reducing the dimensionality as well as mitigating 563 the effects of sketching noise. The performance of our method was evaluated 564 in a series of benchmark tests of FEM simulations that demonstrated sub-565 stantial speed improvements at the cost of a small compromise in accuracy 566 when the stiffness matrix is well conditioned. 567

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