Sensitivity Analysis for Linear Functionals of Solutions to Partial Differential Equations

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Outline

- Model problem
- The method we use to compute stochastic moments of (U, ψ). (such as $E[\cdot]$ and Var$(\cdot)$)
- Error analysis
- Adaptivity
- Numerical examples
- Conclusions and future work

The model problem

Strong form: The Dirichlet Problem with multiple right hand sides, $F_j = \sum_{i=1}^{m} A_i^j v_i(x)$, $v_i \in L^2(\Omega)$, A_i^j random numbers, $j = 1, \ldots, s$, F_j are iid,

$$-\triangle U_j = F_j \quad \text{in } \Omega,$$
$$U_j = 0 \quad \text{on } \Gamma.$$

Weak form: Find $U_j \in V = H_0^1(\Omega)$ such that,

$$(\nabla U_j, \nabla v) = (F_j, v) \quad \text{for all } v \in V.$$

The corresponding dual problem

Strong form: Let $\psi \in L^2(\Omega)$,

$$-\triangle\phi = \psi \quad \text{in } \Omega,$$
$$\phi = 0 \quad \text{on } \Gamma.$$

Weak form: Find $\phi \in V$ such that,

$$(\nabla w, \nabla\phi) = (w, \psi) \quad \text{for all } w \in V.$$

Note that the dual problem is *deterministic*.

Simple observation

Using Green's identity we get,

$$(U_j, \psi) = (\nabla U_j, \nabla \phi) = (F_j, \phi) \quad \text{for } j \in 1 \ldots, s.$$

- We can derive the distribution for (U_j, ψ) by just solving *one* PDE.
- This works as long as the differential operator is linear and deterministic i.e. for a wide range of problems.
- It also works for stochastic initial and boundary condition.

Discretization

Let $V_h \subset V$. We discretize both the primal and the dual using the *same* space,

FEM (primal): Find $U_{h,j} \in V_h$ such that,

$$(\nabla U_{h,j}, \nabla v) = (F_j, v) \quad \text{for all } v \in V_h.$$

FEM (dual): Find $\phi_h \in V_h$ such that,

$$(\nabla w, \nabla \phi_h) = (w, \psi) \quad \text{for all } w \in V_h.$$

Same trick again

Using Green's identity we get,

$$(U_{h,j}, \psi) = (\nabla U_{h,j}, \nabla \phi_h) = (F_j, \phi_h) \quad \text{for } j \in 1, \ldots, s.$$

- We now have a computable approximation of (U_j, ψ) namely (F_j, ϕ_h).
- We are interested in computing stochastic moments of $X_j = (U_j, \psi)$, $m(X)$ cheaply.
- We need error control for both discretization (h) and the number of samples we use to compute the moments ($n \ll s$).

Error estimation

Let $X_j = (U_j, \psi)$ and $X_{h,j} = (F_j, \phi_h)$. Let $m(X)$ denote the exact stochastic moment and let $M(X)$ be an unbiased estimator computed using n realizations of X i.e. $E[M(X)] = m(X)$.
We divide the error into two parts,

$$m(X) - M(X_h) = (m(X_h) - M(X_h)) + (m(X) - m(X_h))$$

- We call the first part *Stochastic error* (n).
- We call the second part *Discretization error* (h).

Stochastic error $m(X_h) - M(X_h)$

Chebyshev inequality:
$P(|Y - E[Y]| \geq \delta) < \text{Var}(Y)/\delta^2$ or by choosing $\delta = \sqrt{\text{Var}(Y)/\epsilon}$,

$$P\left(|Y - E[Y]| < \sqrt{\text{Var}(Y)/\epsilon}\right) \geq 1 - \epsilon.$$

We let $Y = M(X_h)$ and use $E[Y] = E[M(X_h)] = m(X_h)$ to get,

$$P\left(|m(X_h) - M(X_h)| < \sqrt{\text{Var}(M(X_h))/\epsilon}\right) \geq 1 - \epsilon.$$

Example 1: $m(X) = E[X]$

If $m(X) = E[X]$ then $M(X) = \bar{X}$. We have,

$$P\left(|E[X] - \bar{X}| < \sqrt{\text{Var}(\bar{X}_h)/\epsilon}\right) \geq 1 - \epsilon.$$

$$\text{Var}(\bar{X}_h) = \text{Var}\left(\sum_{i=1}^{n} X_{h,j}/n\right) = \text{Var}(X_{h,j})/n.$$

Since F_j are iid X_j and $X_{h,j}$ will also be iid.

$$P\left(|E[X] - \bar{X}| < \sigma/\sqrt{n\epsilon}\right) \geq 1 - \epsilon.$$

Example 2: $m(X) = \mathbf{Var}(X)$

$M(X) = S_n^2(X) = \sum_{j=1}^n (X_j - \bar{X}_j)^2/(n-1)$.
We need to estimate the variance of $S_n^2(X_h)$.

$$\text{Var}(S_n^2(X_h)) = \text{Var}\left(\sum_{j=1}^n (X_{h,j} - \bar{X}_{h,j})^2\right)/(n-1)^2.$$

We assume $(X_{h,j} - \bar{X}_{h,j})^2$ to be almost indep.,

$$\text{Var}(S_n^2(X_h)) \approx \sum_{j=1}^n \text{Var}\left((X_{h,j} - \bar{X}_{h,j})^2\right)/(n-1)^2.$$

Example 2: (cont)

Given $\{X_{h,j}\}_{j=1}^{n}$ we can get a good approximation of Var$((X_{h,j} - \bar{X}_{h,j})^2)$ using the unbiased estimator on this particular sample, lets call it $s_n^2((X_h - \bar{X}_h)^2) \approx$ Var$((X_{h,j} - \bar{X}_{h,j})^2)$.

$$\text{Var}(S_n^2(X_h)) \approx n s_n^2((X_h - \bar{X}_h)^2)/(n-1)^2,$$

so

$$P\left(|\text{Var}(X_h) - S_n^2(X_h)| < \sqrt{C_2/n\epsilon}\right) \geq 1 - \epsilon,$$

where C_2 is computable.

Discretization error $m(X) - m(X_h)$

Remember that,

$$m(X) - m(X_h) = m((F, \phi)) - m((F, \phi_h)).$$

Since ϕ is not known and we only have access to M we need to modify this. Let $\phi_{\gamma h}$, $0 < \gamma < 1$, be an improved version of ϕ_h. Then,

$$m(X) - m(X_h) = M((F, \phi_{\gamma,h})) - M((F, \phi_h))$$
$$+ M((F, \phi)) - M((F, \phi_{\gamma h}))$$
$$+ m((F, \phi)) - m((F, \phi_h)) - M((F, \phi)) + M((F, \phi_h))$$

Example 1: $m(X) = E[X]$

In this case m is linear which means that,

$$m(X) - m(X_h) = E[X - X_h] = E[(F, \phi - \phi_h)]$$
$$= (\bar{F}, \phi - \phi_h) + (E[F] - \bar{F}, \phi - \phi_h)$$
$$= (\bar{F}, \phi_{\gamma h} - \phi_h) + (\bar{F}, \phi - \phi_{\gamma h}) + (E[F] - \bar{F}, \phi - \phi_h).$$

However is this case we have another option.

We could construct a dual problem to take care of the $(\bar{F}, \phi - \phi_h)$-term.

Dual problem for the dual

Let $\chi \in V$ solve,

$$-\triangle \chi = \bar{F} \quad \text{in } \Omega,$$
$$\chi = 0 \quad \text{on } \Gamma.$$

We get the following error representation formula,

$$\begin{aligned}(\phi - \phi_h, \bar{F}) &= (\nabla(\phi - \phi_h), \nabla \chi) \\ &= (\psi, \chi) - (\nabla \phi_h, \nabla \chi) \\ &= (R(\phi_h), \chi - \pi_h \chi).\end{aligned}$$

Example 1: (cont)

The discretization part of the error when $m(X) = E[X]$ consists of two terms,

$$E[X] - E[X_h] = (R(\phi_h), \chi - \pi_h \chi) + (E[F] - \bar{F}, \phi - \phi_h).$$

We can proceed with an interpolation estimate if we assume enough regularity in χ,

$$|E[X] - E[X_h]| \leq C \|h^2 R(\phi_h)\| + |(E[F] - \bar{F}, \phi - \phi_h)|.$$

We can now combine this estimate with the estimate of the stochastic error contribution.

Example 1: Total error estimate

We want to estimate $E[X]-\bar{X}_h$. If we combine the two results we get: the probability that,

$$|E[(U,\psi)]-(\bar{U}_h,\psi)| \leq \sqrt{\text{Var}((F,\phi_h))/(n\epsilon)} + C\|h^2 R(\phi_h)\| + |(E[F]-\bar{F},\phi-\phi_h)|.$$

holds is greater then $1-\epsilon$.

$$|E[(U,\psi)]-(\bar{U}_h,\psi)| \leq C_1/\sqrt{n\epsilon}+C_2h^2, \quad n \sim h^{-4}.$$

In general

For an arbitrary moment m we will have to compute $\phi_{\gamma h}$ and an approximation to Var$(M(X_h))$ in order to get an the following approximate bound:

$$|m(X) - M(X_h)| \leq \sqrt{\text{Var}(M(X_h))/\epsilon} + |M((F, \phi_{\gamma h})) - M((F, \phi_h))|,$$

holds approximately with probability $1 - \epsilon$.

The higher order terms are neglected here.

Same method for related problems 1

Different linear deterministic operator:

$$LU_j = F_j \quad \text{in } \Omega,$$
$$U_j = 0 \quad \text{on } \Gamma.$$

$$L^*\phi = \psi \quad \text{in } \Omega,$$
$$\phi = 0 \quad \text{on } \Gamma.$$

$$(U_j, \phi) = (U_j, L^*\phi) = (LU_j, \phi) = (F_j, \phi).$$

Same method for related problems 2

Stochastic initial condition:

$$\dot{U}_j - \triangle U_j = 0 \quad \text{in } \Omega, \qquad t > 0,$$
$$U_j = 0 \quad \text{on } \Gamma, \qquad t > 0,$$
$$U_j = F_j \quad \text{for } t = 0.$$

$$-\dot{\phi} - \triangle\phi = 0 \quad \text{in } \Omega, \qquad t < T,$$
$$\phi = 0 \quad \text{on } \Gamma, \qquad t < T,$$
$$\phi = \psi \quad \text{for } t = T.$$

Same method for related problems 2

Again we can use that the dual problem is deterministic to get a simple formula to compute the distribution of a linear functional of the solution.

$$(U_j(T), \psi) = (F_j, \phi(0)).$$

This can also be combined with a different deterministic operator.

We can also have a stochastic boundary condition.

Same method for related problems 3

Stochastic boundary condition:

$$-\triangle U_j = 0 \quad \text{in } \Omega,$$
$$-\partial_n U_j = kU_j + F_j \quad \text{on } \Gamma,$$

$$-\triangle \phi = \psi \quad \text{in } \Omega,$$
$$-\partial_n \phi = k\phi \quad \text{on } \Gamma.$$

$$(U_j, \psi) = -\langle F_j, \phi \rangle.$$

Numerical examples: m(X)=E[X]

Stochastic boundary cond., $F_j = -\sin(\pi y) + \delta_j^{[5]}$

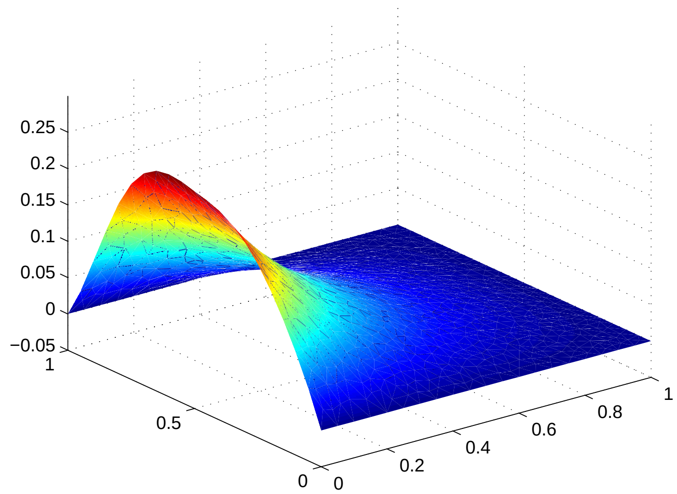

Figure 1: Quasi uniform mesh with meshsize $h \approx 0.05$, $\delta = 0.6$, $k = 0$ on Neumann part.

Test of convergence (h)

Error computed using reference solution, $n_{ref} = 5e5$ and $h_{ref} = 0.01$. We let $\epsilon = 0.05$.

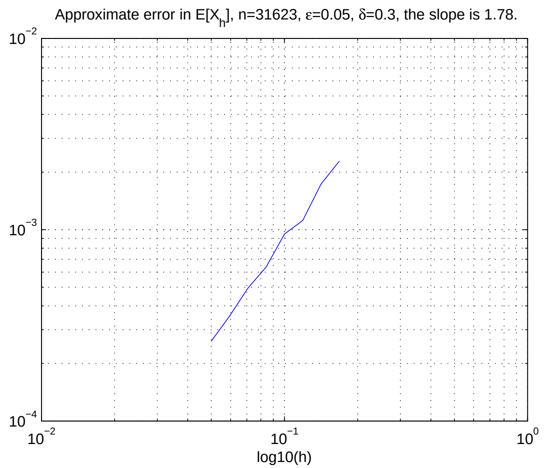

Figure 2: For each h compute ≈ 160 real. of the error using $n \approx 3e4$ and pick the 95% worst value.

Test of convergence (n)

Error computed using reference solution, $n_{ref} = 5e5$ and $h_{ref} = 0.01$. We let $\epsilon = 0.05$.

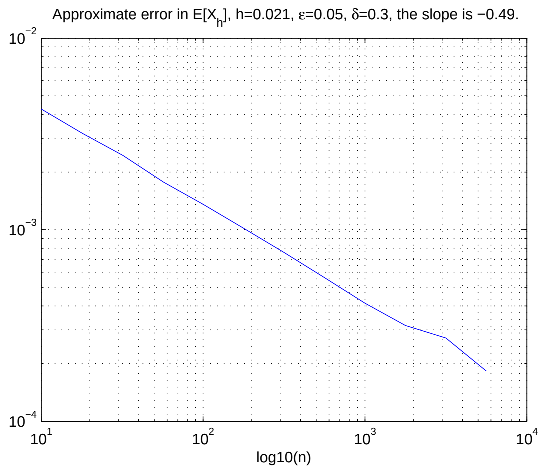

Figure 3: For each n compute $\approx 5e5/n$ real. of the error using $h \approx 0.02$ and pick the 95% worst.

Test of convergence in both h and n

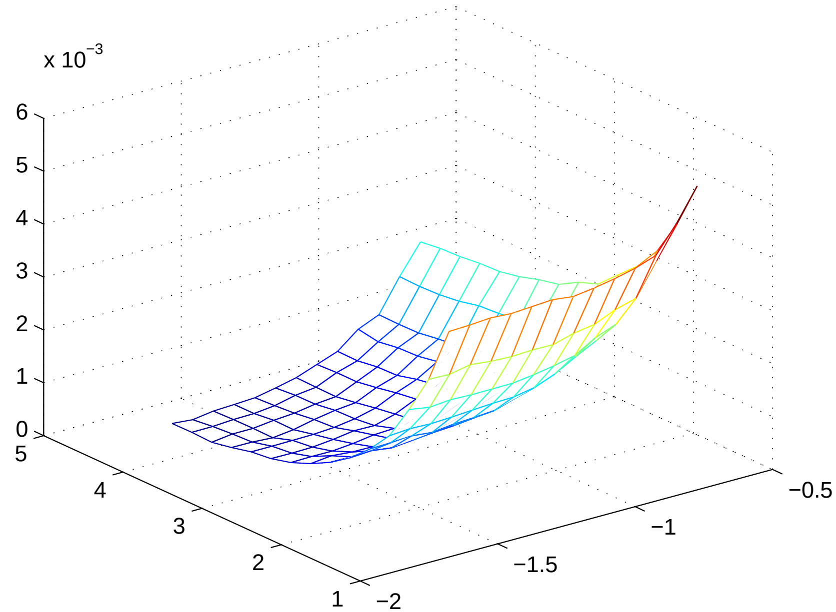

Figure 4: The $1-\epsilon$ probability bound of $|E[X_{h_{ref}}]-\bar{X}_h|$ for different choices of h and n.

Test of convergence in both h and n

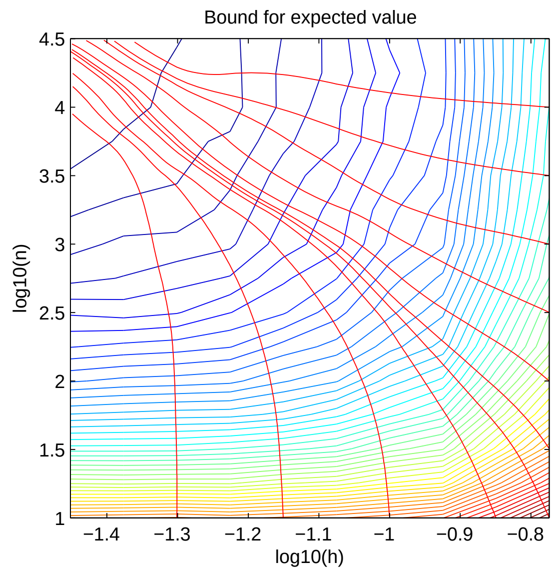

Figure 5: Contour plot with steepest decent paths indicating the dependence between h and n when trying to minimize the error.

The error bound (no reference)

We let $n = 31623$ and vary h between $0.05 \le h \le 0.168$.

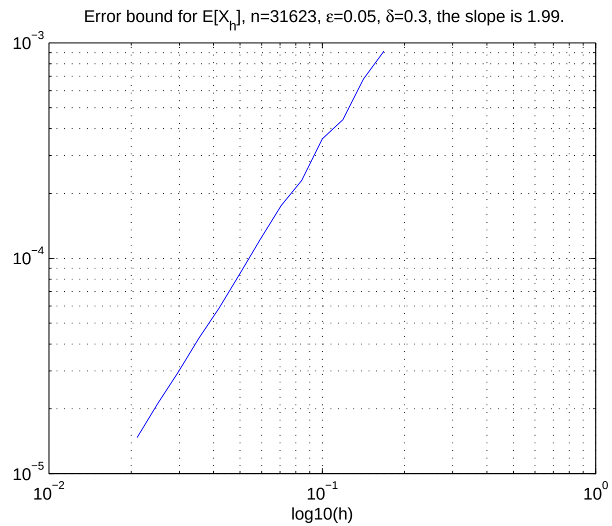

Figure 6: We note that the $1-\epsilon$ bound of $|\bar{X} - \bar{X}_h|$ approximately depends on h^2.

The error bound (no reference)

Let $h = 0.021$ and compute the bound of the stochastic contribution of the error.

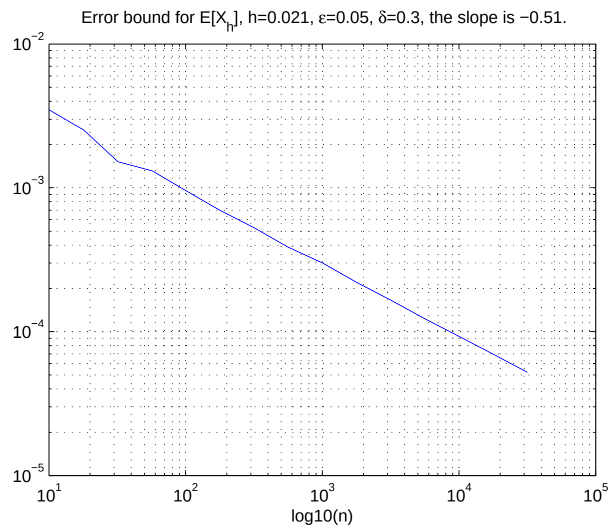

Figure 7: We note that the $1-\epsilon$ bound of $|\bar{X}-\bar{X}_h|$ approximately depends on $1/\sqrt{n}$.

Adaptivity in h and n

1. Choose ϵ, TOL, $r > 1$, $h = h_{st}$, and $n = n_{st}$.
2. Compute the solutions $X_{h,j}$, $1 \leq j \leq n$.
3. Compute $S = \sigma/\sqrt{n\epsilon}$.
4. Compute $D = (\psi, \chi - \pi_h \chi) - (\nabla \phi_h, \nabla(\chi - \pi_h \chi)) - \langle k\phi_h, \chi - \pi_h \chi \rangle$.
5. If $D + S < TOL$ stop.
6. If $D > rS$ then let $h := h/r$ and $n := n$. If $S < rD$ then let $h := h$ and $n := r \cdot n$. Otherwise $h := h/r$ and $n := n \cdot r$.

Adaptivity in h and n

Let $\epsilon = 0.05$, $r = 1.5$, $TOL = 5 \cdot 10^{-5}$, (rel. error less then 0.1%), $h_{st} = 0.2$, and $n_{st} = 40$.

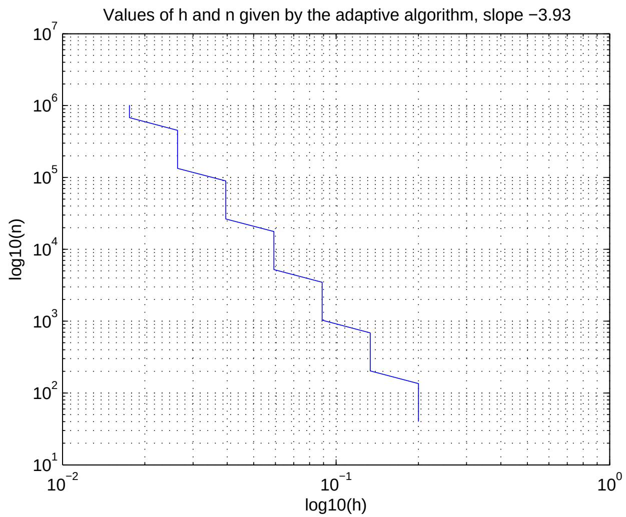

Figure 8: We see clearly how the algorithm enforces $n \sim h^{-4}$.

Bound vs. true error (reference)

Error comp. to ref. solution and error bound after each iterations in the adaptive algorithm.

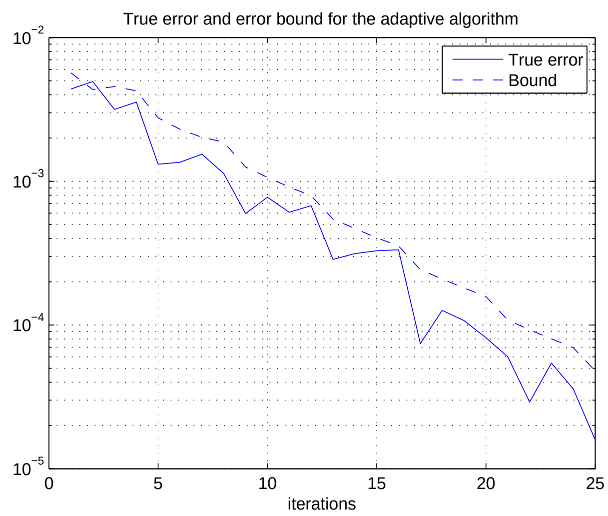

Figure 9: Neglecting the higher order term does not cause any trouble in this example.

Numerical examples: m(X)=Var(X)

We start with the h-dependence.

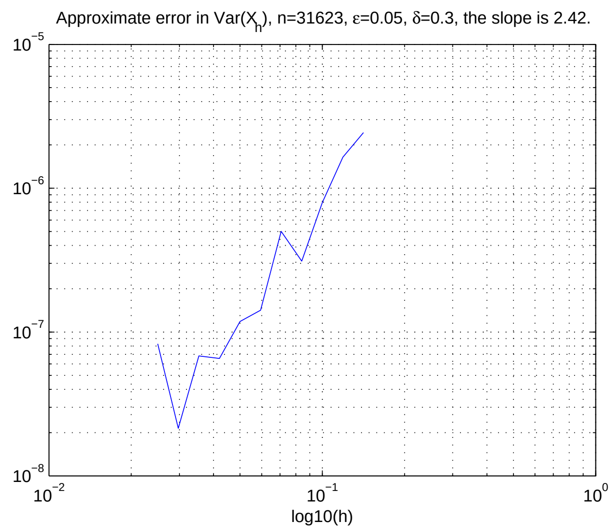

Figure 10: We note that the $1-\epsilon$ probability bound of $|S^2_{n_{ref}}(X_{h_{ref}}) - S^2_n(X_h)|$ depends roughly on $h^{2.4}$.

Convergence for Var (n)

The n-dependence.

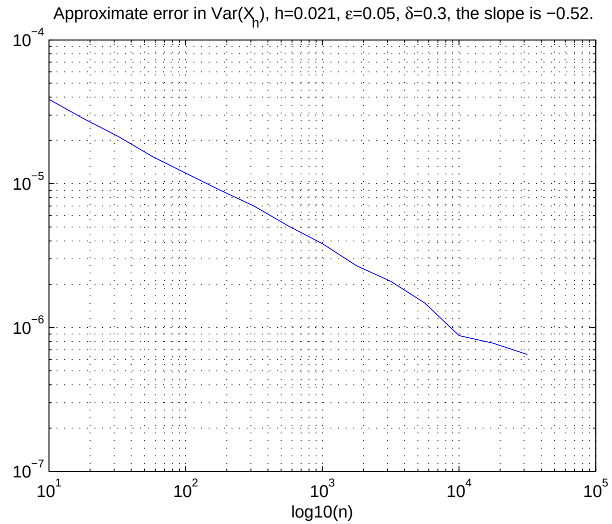

Figure 11: We note that the $1-\epsilon$ bound of $|S_n^2(X_{h_{ref}}) - S_{n_{ref}}^2(X_h)|$ appr. depends on $1/\sqrt{n}$.

Test of convergence in h and n

Next we study the surface we get from varying both h and n.

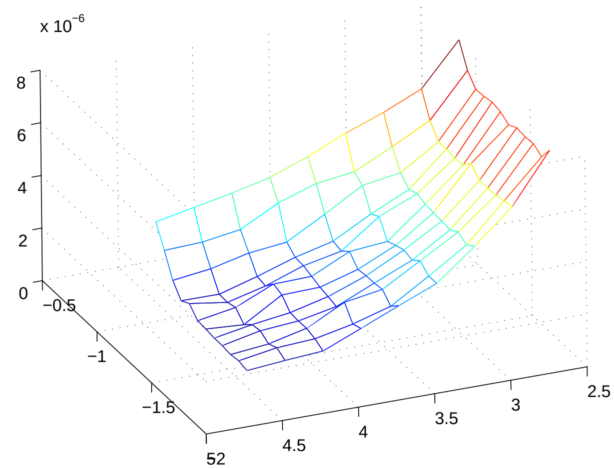

Figure 12: The $1-\epsilon$ probability bound of $|S_n^2(X_{h_{ref}}) - S_n^2(X_h)|$ versus h and n.

Error bound, h-part no reference

The h-dependent part, $M(X_{\gamma h}) - M(X_h)$.

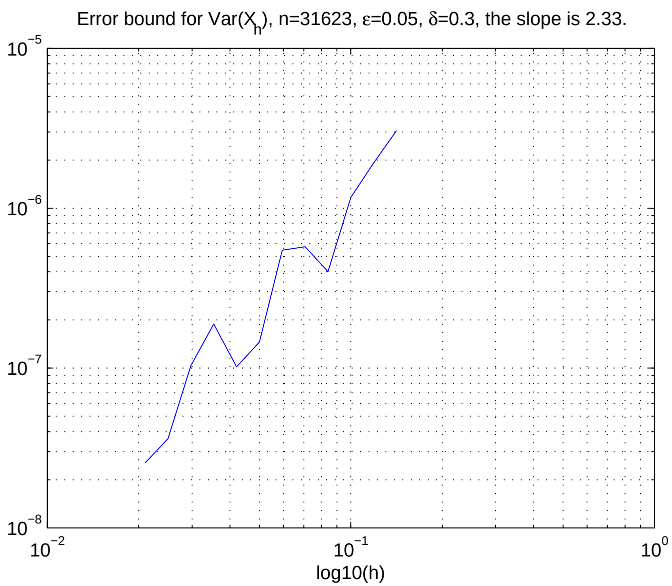

Figure 13: The $1-\epsilon$ probability bound of $|\text{Var}(X) - S_n^2(X_h)|$.

Error bound, n-part no reference

The n-dependency is again easier to capture.

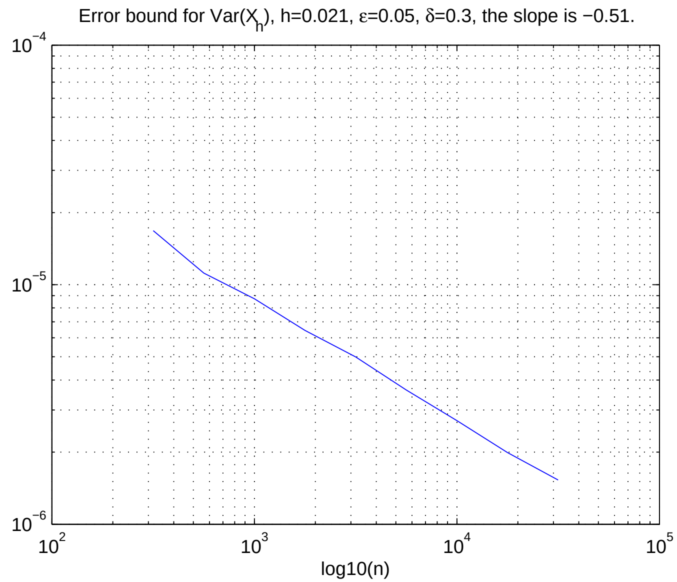

Figure 14: We note that the $1-\epsilon$ bound of $|\mathrm{Var}(X) - S_n^2(X_h)|$ depends on $1/\sqrt{n}$.

Error bound varying both h and n

We plot the surface of the bound we get by varying h and n.

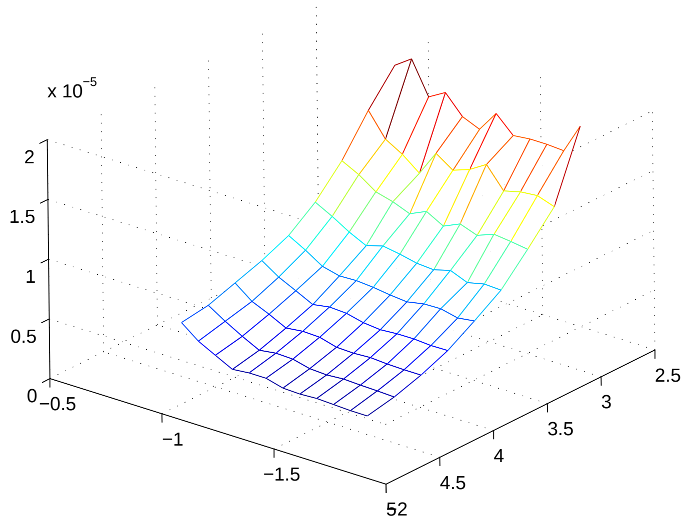

Figure 15: The error bound of $|\mathrm{Var}(X) - S_n^2(X_h)|$.

Efficiency

Efficiency of the estimate.

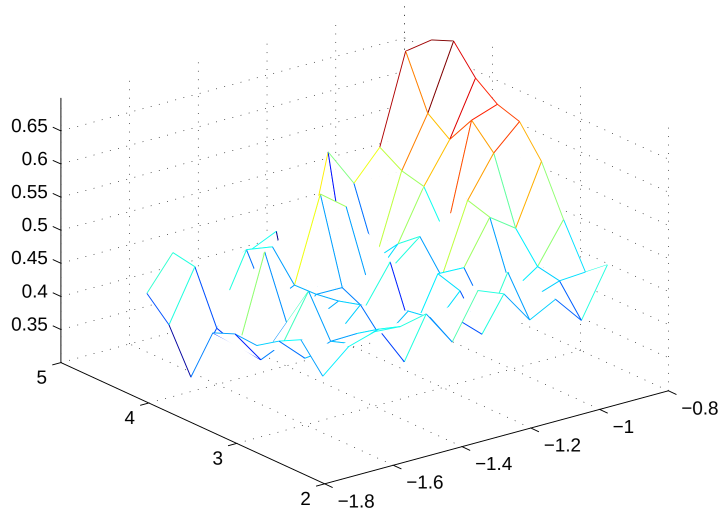

Figure 16: The error compared to the reference solution divided by the error bound.

Adaptive algorithm

Let $\epsilon = 0.05$, $r = 1.5$, $TOL = 10^{-7}$, (rel. error $< 0.2\%$), $h_{st} = 0.2$, and $n_{st} = 10^3$.

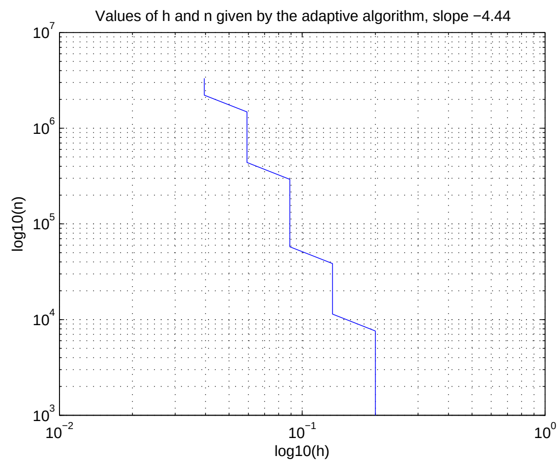

Figure 17: We see how the algorithm gives us roughly $n \sim h^{-4.4}$.

Error bound vs. "true" error

We compare the error bound with the error compared to a reference solution.

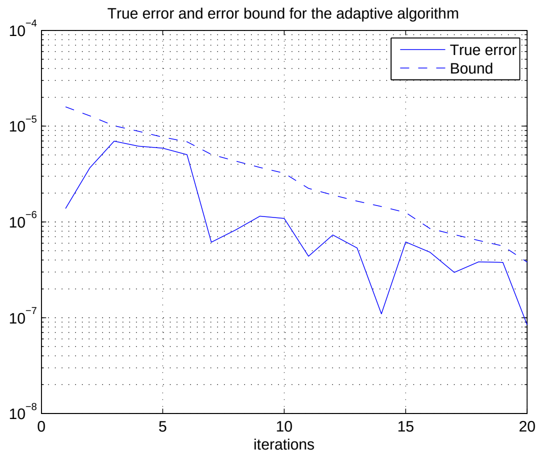

Figure 18: The solid line is error compared to a ref. sol. and the dashed line is the error bound.

Conclusion and future work

- Cheap method for computing arbitrary stochastic moments of linear functionals of solution to a wide class of linear PDE’s.
- Error analysis that takes both the traditional discretization error and *stochastic error* into account.
- Numerical results that agrees with theory.
- At the moment we work on stochastic diffusion coefficient in the Poisson equation.