## Application-specific quadrature for fast evaluation of parameterized inner products with noisy data

#### Scott Field

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Joint work with Harbir Antil (George Mason), Priscilla Canizares (Cambridge), Frank Herrmann (UMD), Jonathan Gair (Cambridge), Ricardo Nochetto, (UMD), Manuel Tiglio (UMD).

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#### Introduction

Reduced order quadratures Experiments and applications Parameterized integration Gravitational wave parameter estimation

### Outline

#### Introduction

- Reduced order quadratures
- Experiments and applications

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Parameterized integration Gravitational wave parameter estimation

## Numerical quadrature

Consider the problem of integrating a function in 1 spatial dimension

$$\int_{\Omega} f(x) W(x) dx \approx \sum_{i=1}^{N} f(x_i) \omega_i$$

Finding quadrature points  $x_i$  and weights  $\omega_i$  is well-studied

- ▶ Is f smooth? Use Gaussian quadratures for a standard W
- ▶ Is f non-smooth? Use trapezoidal or Simpson's rule
- Error estimator? Gauss-Kronrod rule

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### Parameterized integrations

Consider the parameterized problem in 1 spatial dimension

$$\langle f,g\rangle(\mu,\nu) = \int_{\Omega} f^*(x;\mu)g(x;\nu)W(x)dx \approx \sum_{i=1}^N f^*(x_i;\mu)g(x_i;\nu)\omega_i$$

computed with any ordinary quadrature rule with an integrand  $f^*(x)g(x)$ Outlook

- ▶ If  $10^6$  values of  $(\mu, \nu)$  are needed, each  $\approx$  1s, our code takes 12 days!
- ► We might design a custom quadrature rule tailored to our functions
- Invest time to build worthwhile if its faster to use (and reuse)

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### Difficulties with parameterized integration

$$\langle f,g\rangle(\mu,\nu) = \int_{\Omega} f^*(x;\mu)g(x;\nu)W(x)dx$$

Existing numerical quadrature rules could be expensive whenever...

- $f(x; \mu)$  or  $g(x; \nu)$  are not well approximated by standard functions
- $f(x; \mu)$  or  $g(x; \nu)$  highly oscillatory or different length scales
- $f(x; \mu)$  is a stream of noisy data s(x), sampling dictated by experiment
- W(x) is something strange, perhaps empirically derived

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### Observations and strategies

$$\langle f,g\rangle(\mu,\nu) = \int_{\Omega} f^*(x;\mu)g(x;\nu)W(x)dx$$

Some common situations...

- Needs to be computed for many values of  $(\mu, \nu)$
- Won't know ahead of time which parameters to compute for
- Could be a serial procedure: selected  $(\mu_i, \nu_i)$  depends on previous i-1
- If  $g(x; \nu) = s(x)$  noisy data, integration often depends smoothly on  $\mu$

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### Observations and strategies

$$\langle f,g\rangle(\mu,\nu) = \int_{\Omega} f^*(x;\mu)g(x;\nu)W(x)dx$$

Plan of attack...

- Invest effort to build an application-specific quadrature rule offline
- Once built it is reused *online*, for example when new data is available
- If  $\langle f, g \rangle$  has smooth parametric dependence we expect fast, accurate rule

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### Motivations

Gravitational waves emitted from two orbiting black holes. These sources could be in our galaxy or another one far, far away.



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Parameterized integrations in gravitational wave (GW) data analysis

- 1. A GW detector records some signal  $s(t) = h(t; \lambda) + n(t)$
- 2. Noise  $|n(t)| \gg |h_{\lambda}(t)|$
- 3. Parameter estimation by correlating signal with model  $h(t; \mu)$  to recover parameter  $\lambda$
- 4. Analysis can take hours to many months depending on data and model

1. Noise free signal  $h(t; \lambda)$ 



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2. Observed signal s(t)



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3. To recover  $\lambda$  multiple evaluations of

$$\int_{f_{\rm low}}^{f_{\rm high}} s^*(f) h(f;\mu) W(f) df$$

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and W(f) describes detector noise

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#### 4. This may take a while



Parameterized integration Gravitational wave parameter estimation

### Preview of talk

- Algorithms to build application-specific quadrature rules for generic, parameterized integrals
- Work largely motivated by bottlenecks encountered in data analysis studies
- Examples typically draw from GW physics, however approach is general

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## Problem Formulation

#### Parametrized Functions

Let

$$\mathcal{F} := \{h_{\mu} : \Omega \to \mathbb{C} \mid \mu \in \mathcal{P}, h_{\mu} \in \mathcal{C}\}$$

be a set of parametrized functions where  $\Omega$ ,  $\mathcal{P}$  denote the "physical" and parameter domains and  $\mathcal{F}$  denotes a compact subset of a Hilbert space  $\mathcal{H} \supset \mathcal{F}$ .

- $h_{\mu}$  could be closed-form, solutions to ODEs or PDEs
- ▶ In data analysis context  $h_{\mu}$  is the parameterized model

#### Inner Product Computation

• Given two arbitrary parameters  $\mu_1, \mu_2 \in \mathcal{P}$ , consider

$$\langle f,g 
angle \left( \mu_{1},\mu_{2} 
ight) = \int_{\Omega} f_{\mu_{1}}^{*}(x)g_{\mu_{2}}(x)W(x)dx$$

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### Introduction to reduced order quadratures (ROQ)

### ROQ roadmap

1. We have an existing quadrature rule and a set of functions  $\ensuremath{\mathcal{F}}$ 

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### Introduction to reduced order quadratures (ROQ)

### ROQ roadmap

- 1. We have an existing quadrature rule and a set of functions  $\ensuremath{\mathcal{F}}$
- 2. Find an accurate and compact basis to represent any element of  $\mathcal{F}$ . The basis will be a non-standard, application-specific one

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- 3. Find points in the physical domain  $\boldsymbol{\Omega}$  for good integration
  - Points could be a subset of the existing quadrature rule
  - Accurate and stable (recall Newton-Cotes becomes ill-conditioned)

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- 3. Find points in the physical domain  $\boldsymbol{\Omega}$  for good integration
  - Points could be a subset of the existing quadrature rule
  - Accurate and stable (recall Newton-Cotes becomes ill-conditioned)
- 4.  $\{x_i, \omega_i\}_{i=1}^N \to \{X_i, \omega_i^{\text{ROQ}}\}_{i=1}^n$ . Typically  $n \ll N$ .
- Algorithms/framework draw from recent developments in model order reduction

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## Approximations

Approximation of parameterized functions  $\mathcal{F}$  with an *n*-dimensional space  $X_n$ 

$$\sup_{h_{\mu}\in\mathcal{F}} \inf_{f\in X_n} \|h_{\mu} - f\| \le \epsilon$$

where  $\epsilon$  is a user defined approximation tolerance ( $\approx 10^{-6}$ )

- Non-adaptive approximations
  - Space  $X_n$  fixed and independent of  $\mathcal{F}$
  - ► Example: X<sub>n</sub> degree n polynomials (Gaussian quadratures)
- Adaptive approximations
  - Space  $X_n$  tailored to  $\mathcal{F}$
  - Example: Basis of  $X_n$  drawn from  $\mathcal{F}$  (reduced order quadratures)

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### When to seek adaptive approximations?

- Time invested to find adaptive approximations worthwhile
  - Expect to reuse information
- Non-adaptive approximations are poor
- High evaluation cost  $h_{\mu}(x_i)$  at each  $x_i \in \Omega$ 
  - Even moderately fewer x<sub>i</sub> will be useful

When will adaptive approximations converge quickly??

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#### Kolmogorov *n*-width of $\mathcal{F}$ in $\mathcal{H}$

$$d_n(\mathcal{F};\mathcal{H}) := \inf_{\dim X_n \leq n} \sup_{h_\mu \in \mathcal{F}} \inf_{f \in X_n} \|h_\mu - f\| = \inf_{\dim X_n \leq n} \sup_{h_\mu \in \mathcal{F}} \|h_\mu - \mathcal{P}_n h_\mu\| ,$$

measures error of the best n-dimensional subspace  $X_n \subset \mathcal{H}$  approximating  $\mathcal{F}$ Orthogonal projection  $\mathcal{P}_n : \mathcal{F} \to X_n$ 

$$h_{\mu} \approx \mathcal{P}_n h_{\mu} := \sum_{i=1}^n \langle e_i, h_{\mu} \rangle e_i ,$$

 $\mathcal{P}_n h_\mu$  is best representation of  $h_\mu$  in  $X_n$  and  $\{e_i\}_{i=1}^n$  an orthonormal basis of  $X_n$ 

Bottleneck: Sadly, finding  $X_n$  is in general not possible!

### Approximate solution to the *n*-width problem

#### 1. Sample the continuum

Define *training set* through sampling at parameter points  $\mathcal{T}_{\mathcal{K}} = \{\mu_i\}_{i=0}^{\mathcal{K}}$ 

$$\mathcal{F}_{\mathcal{K}} = \{h_{\mu} \in \mathcal{F} : \mu \in \mathcal{T}_{\mathcal{K}}\}$$

Note: Sampling must be dense enough

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Note: Sampling must be dense enough

### 2. Greedy strategy

Find  $F_n \approx \mathcal{F}_K$  by solving *n* easy problems

- Given  $F_i$  the algorithm optimally chooses  $F_{i+1}$  and continues to  $F_n$
- ▶ Sequence of hierarchical spaces are constructed  $F_1 \subset F_2 \subset ... \subset F_n$

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# Greedy algorithm (setup)

**Goal**: Find  $F_n \approx \mathcal{F}$ 

- 1. Choose a parameter  ${\mathcal P}$  and physical  $\Omega$  domains
- 2. Sample continuum  $\mathcal{P}$  with *dense* training set  $\mathcal{T}_{\mathcal{K}} = \{\mu_i\}_{i=0}^{\mathcal{K}}$
- 3. Initialize algorithm with random  $\mu_1$  and let  $F_1 = \operatorname{span}\{h_{\mu_1}\}$

To go from  $F_i$  to  $F_{i+1}$ ...

Model's n-width and the greedy algorithm: the basis Empirical interpolation: the nodes Building an ROQ

### Greedy algorithm

Define greedy error  $\sigma_i(\mathcal{F}_K; \mathcal{H}) := \sup_{\mu \in \mathcal{T}_K} \|h_\mu - \mathcal{P}_i h_\mu\|$ 

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## Greedy algorithm

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While  $\sigma_i(\mathcal{F}_{\mathcal{K}};\mathcal{H}) \geq \mathrm{Tol}$ 

 $i \rightarrow i + 1$ 

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### $i \rightarrow i+1$

1. For all  $\mu \in \mathcal{T}_{\mathcal{K}}$  compute  $||h_{\mu} - \mathcal{P}_{i}h_{\mu}||$ 

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## Greedy algorithm

11.4 Define greedy error  $\mu$ 

$$\sigma_i(\mathcal{F}_{\mathcal{K}};\mathcal{H}) := \sup_{\mu \in \mathcal{T}_{\mathcal{K}}} \|h_{\mu} - \mathcal{P}_i h_{\mu}$$

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- 1. For all  $\mu \in \mathcal{T}_K$  compute  $||h_{\mu} \mathcal{P}_i h_{\mu}||$
- 2. Find the parameter  $\mu_{i+1}$  which maximizes the error of step 1

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## Greedy algorithm

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3. Let 
$$h_{i+1} = h_{\mu_{i+1}}$$
 and  $F_{i+1} = \operatorname{span}\{h_1, ..., h_{i+1}\}$ 

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## Greedy algorithm

U.L. Define greedy error

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- 3. Let  $h_{i+1} = h_{\mu_{i+1}}$  and  $F_{i+1} = \operatorname{span}\{h_1, \dots, h_{i+1}\}$

**Output:** Collection of points  $\{\mu_i\}_{i=1}^n$  and corresponding basis  $\{h_i\}_{i=1}^n$ **Result**:  $F_n = \operatorname{span}\{h_i\}_{i=1}^n$  approximates training space  $\mathcal{F}_K$  up to Tol

$$d_n(\mathcal{F};\mathcal{H}) \leq C e^{-c_0 n^{lpha}} \quad o \quad \sigma_n(\mathcal{F};\mathcal{H}) \leq \sqrt{2C} e^{-c_1 n^{lpha}}$$

where C,  $c_0$ ,  $\alpha$ , and  $c_1 := 2^{-1-2\alpha}c_0$  are positive constants.

$$d_n(\mathcal{F};\mathcal{H}) \leq C e^{-c_0 n^{lpha}} \quad o \quad \sigma_n(\mathcal{F};\mathcal{H}) \leq \sqrt{2C} e^{-c_1 n^{lpha}}$$

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Remarks

 $\triangleright$  F<sub>N</sub> found through greedy algorithm nearly optimal compared to best space

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#### Remarks

- $F_N$  found through greedy algorithm nearly optimal compared to best space
- If we define an *M*-by-*K* matrix A = [h<sub>µ1</sub>(**x**),..., h<sub>µK</sub>(**x**)] the greedy selects n columns from A which serve as a low-rank approximation

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#### Remarks

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- If we define an *M*-by-*K* matrix A = [h<sub>µ1</sub>(**x**),..., h<sub>µK</sub>(**x**)] the greedy selects n columns from A which serve as a low-rank approximation
- Basis identified through greedy allows ROQ error to be controlled by n-widths thanks to Binev, DeVore, et al

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## Quadrature nodes

To complete the ROQ rule we must select nodes from physical domain  $\boldsymbol{\Omega}$ 

- ▶ What are good points for integrating in space *F<sub>n</sub>*?
- In data analysis applications points *cannot* be freely drawn from  $\Omega$
- Hierarchical nodal set advantageous
  - Faster to find
  - Leads to embedded ROQ rules

Preview: We will find *n* nodes and derive an interpolatory quadrature formula
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Recall a greedy algorithm has identified a basis  $\{e_i\}_{i=1}^n$ 

- Empirical interpolant
  - ► If we know n "good" nodes

$$\{X_i\}_{i=1}^n \subset \Omega$$

then any  $h_{\mu} \in \mathcal{F}$  can be written as

$$\mathcal{I}_n[h_\mu](x) := \sum_{i=1}^n c_i(\mu) e_i(x)$$

where the  $c_i$  coefficients are solutions to the interpolation problem

$$\mathcal{I}_n[h_\mu](X_k) = h_\mu(X_k), \qquad \forall \ k = 1, \dots, n.$$

► ROQ rule is found by some version of " $\int_{\Omega} \mathcal{I}_n[h_\mu](x) dx$ "

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# Empirical Interpolation Method<sup>1</sup> (EIM)

- ► For application-specific bases where points are not known a-priori
- Algorithm selects interpolation points through a greedy criteria

Training set of physical points Let  $\vec{x} = (x_1, x_2, \dots, x_N)^T$  denote a vector of points where the set

$$\{x_i\}_{i=1}^N \subset \Omega$$

Goal: *n* points  $\{X_i\}_{i=1}^n \subset \{x\}_{i=1}^N$  such that

$$\|h_{\mu} - \mathcal{I}_n[h_{\mu}]\| \approx \sigma_n(\mathcal{F};\mathcal{H})$$

Recall best L2 approximation:  $\|h_{\mu} - \mathcal{P}_n h_{\mu}\| \leq \sigma_n(\mathcal{F}; \mathcal{H})$ 

<sup>1</sup>Barrault 2004, Maday 2009, Chaturantabut 2009, Sorensen 2009 - < = > < = >

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Input: *n* evaluated basis functions  $\{\vec{e}_i\}_{i=1}^n$ , where  $\vec{e}_i = e_i(\vec{x})$ 

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 $i = \operatorname{argmax} |\vec{e}_1|$  **Comment:** argmax returns the index of its largest entry. Set  $X_1 = x_i$ 

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- $i = \operatorname{argmax} |\vec{e}_1|$  **Comment:** argmax returns the index of its largest entry. Set  $X_1 = x_i$
- For  $j = 2 \rightarrow n$  do
  - 1. Find  $\mathcal{I}_{j-1}[e_j](\vec{x})$

 $i = \operatorname{argmax} |\vec{e}_1|$  **Comment:** argmax returns the index of its largest entry. Set  $X_1 = x_i$ 

For  $j = 2 \rightarrow n \text{ do}$ 

- 1. Find  $\mathcal{I}_{j-1}[e_j](\vec{x})$
- 2. Compute the point-wise error  $\vec{r} = \mathcal{I}_{j-1}[e_j](\vec{x}) \vec{e}_j$

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- 3.  $i = \operatorname{argmax} |\vec{r}|$
- 4. Set  $X_j = x_i$

**Output**: *n* points  $\{X_i\}_{i=1}^n \subset \{x_i\}_{i=1}^N$ 

### Interpolation Error Estimate

Let the set of greedy (reduced) basis  $\{e_i\}_{i=1}^n$  be orthonormal and  $\mathcal{P}_n h_\mu \in F_n$  be the optimal approximation of  $h_\mu$  with respect to the  $L^2$ -norm. Then for every  $\mu \in \mathcal{P}$ 

$$\|h_{\mu} - \mathcal{I}_{n}[h_{\mu}]\| \leq \Lambda_{n} \|h_{\mu} - \mathcal{P}_{n}h_{\mu}\| \leq \Lambda_{n}\sigma_{n}(\mathcal{F};\mathcal{H})$$

where  $\Lambda_n = || \mathcal{I}_n ||_2$  is a Lebesgue-like constant

- $\Lambda_n$  is computable once basis and nodes are known
- No bounds on  $\Lambda_n$ 's growth with n
- Slow growth observed in practice

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#### Standard quadrature

• Let  $\{\alpha_i, x_i\}_{i=1}^N$  denote quadrature weights and points then

$$\int_{\Omega} h_{\mu}(x) dx \approx \sum_{i=1}^{N} \alpha_i h_{\mu}(x_i)$$

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## Standard quadrature

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$$\int_{\Omega} h_{\mu}(x) dx \approx \sum_{i=1}^{N} \alpha_i h_{\mu}(x_i)$$

#### Reduced order quadrature

- The set  $\mathcal{F}$  is approximated by an *n*-dim space  $F_n = \operatorname{span}\{e_i\}_{i=1}^n$
- ▶ EIM points  $\{X_i\}_{i=1}^n$  are accurate and well conditioned for interpolation in  $F_n$

$$\sum_{i=1}^{N} \alpha_i h_{\mu}(x_i) \approx \sum_{i=1}^{N} \alpha_i \mathcal{I}_n[h_{\mu}](x_i) = \sum_{i=1}^{n} \omega_i^{ROQ} h_{\mu}(X_i)$$

Numerical experiments show  $n \ll N$ 

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#### Define

$$I_{c} = \int_{\Omega} h_{\mu}(x) dx, \quad I_{d} = \sum_{i=1}^{N} \alpha_{i} h_{\mu}(x_{i}), \quad I_{ROQ} = \sum_{i=1}^{n} \omega_{i}^{ROQ} h_{\mu}(X_{i})$$

#### ROQ error estimates

Let  $\sigma_n(\mathcal{F}; \mathcal{H}) \leq \epsilon$  then  $\forall h_\mu \in \mathcal{F}$ 

$$|I_{d} - I_{ROQ}| < \sigma_{n}(\mathcal{F}; \mathcal{H})|\Omega|\Lambda_{n}\|h_{\mu}\|_{d} < \epsilon |\Omega|\Lambda_{n}\|h_{\mu}\|_{d}$$

where  $\sigma_n$  is the greedy error,  $\epsilon$  an error tolerance, and  $\Lambda_n = \|\mathcal{I}_n\|_2$ 

$$|I_{c} - I_{ROQ}| < |I_{c} - I_{d}| + \epsilon |\Omega| \Lambda_{n} ||h_{\mu}||_{d}.$$

#### Remarks

- ROQ converges to I<sub>d</sub> with same rate as n-width
- ▶ If  $I_d \approx I_c$  then convergence to exact result with same rate like *n*-width

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Introduction	Model's n-width and the greedy algorithm: the basis
Reduced order quadratures	Empirical interpolation: the nodes
Experiments and applications	Building an ROQ

## Noisy data s

$$\langle s, h_{\mu} \rangle \approx \sum_{i=1}^{N} \alpha_i s^*(x_i) h_{\mu}(x_i) \approx \sum_{i=1}^{N} \alpha_i s^*(x_i) \mathcal{I}_n[h_{\mu}](x_i) = \sum_{i=1}^{n} \omega_i^{ROQ} h_{\mu}(X_i)$$

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#### Noisy data s

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Parameterized products

$$\int_{\Omega} h_{\mu_i}^*(x) h_{\mu_j}(x) dx$$

• Approximation of  $\widetilde{\mathcal{F}} = \{h_{\mu_i}^* h_{\mu_j} \mid h_{\mu_i}, h_{\mu_j} \in \mathcal{F}\}$ 

- Two-step greedy leads to significantly faster offline building of basis
  - ▶ Training set for  $\widetilde{\mathcal{F}}$  uses greedy points found from  $F_n \approx \mathcal{F}$

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# A few considerations

## Implementing the rule

- Finding basis and points could be costly save output
- Someone gives you a good quadrature rule before deriving ROQ

## Typical applications

- ROQ rule will be used over and over
  - Cost of building basis likely to outweigh single use
- > You don't know what parameters are ahead of time (e.g. data analysis)
- ▶ Naive quadrature has too many degrees of freedom (e.g. data analysis)
- Parameters drawn from continuum
  - If you know the parameters, store the results to file!
- Functions smooth ROQ converges exponentially fast

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Introduction Reduced order quadratures Experiments and applications

Results: Comparison with Gaussian quadrature Results: GW parameter estimation

## Outline

## Introduction

Reduced order quadratures

Experiments and applications

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Experiment setup

#### Results: Comparison with Gaussian quadrature Results: GW parameter estimation

## Continuum

•  $x \in [-1,1]$  and weight W(x) = 1

## Discrete quadrature

24-point Gaussian quadrature

## Reduced order quadrature

- > 24 ROQ basis: Legendre polynomials, no greedy algorithm used
- ▶ 24 ROQ points: Subset of 1000 equidistant points sampling the basis

#### Point and weight distribution



Top: Weight  $\omega_k$  and node  $\{x_i\}$  distributions for each 24-point rule Bottom: Quadrature node locations only

## Conditioning of quadrature

- Negative weights can lead to poorly conditioned quadrature
- ▶ *n*-point ROQ rule for  $n \in [2, 200]$



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ROQ for parameterized inner products with noisy data

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Let  $\mu_1, \mu_2 \in [-.1, .1]$  and consider integrals in 1 and 2 dimensions

$$\int_{-1}^{1} \left[ \left( x - \mu_1 \right)^2 + 0.1^2 \right]^{-1/2} \qquad \int_{-1}^{1} \int_{-1}^{1} \left[ \left( x - \mu_1 \right)^2 + \left( y - \mu_2 \right)^2 + 0.1^2 \right]^{-1/2}$$



- ROQ rule built from 150-point (for 1D) or 150<sup>2</sup>-point (for 2D) GQ rule.
- 2D GQ rule from tensor product grids
- ROQ nodal set formed by scattered point distributions tailored to the problem

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# Gravitational waves (GWs)





Courtesy: NASA GSFC

- > Pair of orbiting black holes and/or neutron stars inspiral, merge, and ringdown
- Parameters of the binary system: objects' masses (2 parameters), spins (6 parameters), and location/orientation in sky/detectors (8 parameters)

## Gravitational wave detectors

- In absence of GWs the distance between two points is L
- A passing gravitational wave h(t) causes small  $\Delta L$  changes in length L.



Before GW passes by this ring of point masses has a radius *L* 



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## Gravitational wave detectors

- In absence of GWs the distance between two points is L
- A passing gravitational wave h(t) causes small  $\Delta L$  changes in length L.



Single frequency, cross polarization  $h(t) = h_x \sin(\omega t - kz)$ 

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## Gravitational wave detectors

- In absence of GWs the distance between two points is L
- GW h(t) causes small  $\Delta L$  change in length Expect  $h(t) \propto \frac{\Delta L}{L} \leq 10^{-20}$



<sup>2</sup>Fig. by Lee Lindblom

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## Gravitational wave detectors

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<sup>3</sup>Fig. by Lee Lindblom

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## GW parameter estimation

- A detector alerts us to a signal in noisy data
- Correlate data with GW model to extract the physical parameters

## Difficulties

- Model  $h_{\mu}(t)$  described by high dimensional parameter space
- ▶ Data  $s(t_i) = h_\lambda(t_i) + n(t_i)$  is a long time series,  $\lambda$  true parameter
- N equally spaced samples;  $N = (\text{observation time}) \times (\text{sampling rate})$ 
  - Ex: 32s at 4096Hz suggests  $N \approx 130,000$  samples
- Cost to process data scales with N, dominated by evaluating model  $h_{\mu}(t)$

# GW Bayesian parameter estimation (I)

The (posterior) probability distribution function provides complete information about the parameters of the signal and is given by

 $p(\mu|s) \propto P(s|\mu)$ 

- $p(\mu|s)$  is probability of parameters  $\mu$  given data s
- $P(s|\mu)$  is the *likelihood* that data *s* described by a particular  $\mu$
- ► For Gaussian noise the likelihood is

$$\mathcal{P}\left(s|\mu
ight)\propto\exp\left(-\chi^{2}/2
ight),\quad\chi^{2}=\left\langle s(f)-h_{\mu}\left(f
ight),s(f)-h_{\mu}\left(f
ight)
ight
angle$$

which features Fourier transform of s(t) and  $h_{\mu}(t)$ 

 $\blacktriangleright$  Parameter estimation cost dominated by evaluation of  $\chi^2$ 

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## GW Bayesian parameter estimation (II)

## Markov chain Monte Carlo (MCMC)

- We want to compute probability  $p(\mu|s)$
- MCMC algorithms sample  $p(\mu|s)$ , efficient for high dimensional problems
- MCMC sequentially selects points, each requires evaluation of  $\chi^2$
- Between hours and a year for algorithm to run!

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## Notice

$$\chi^2 = \langle \pmb{s}, \pmb{s} 
angle + \langle \pmb{h}_\mu, \pmb{h}_\mu 
angle - 2 \Re \langle \pmb{s}, \pmb{h}_\mu 
angle$$

- $\langle s, s \rangle$  computed once
- $\langle h_\mu, h_\mu 
  angle$  has simple (often closed-form) expression

## Standard computation

$$\langle s, h_{\mu} \rangle \approx \Delta f \sum_{i=0}^{N} s(f_i) h_{\mu}^*(f_i)$$

where N is the number of data samples

- Widely (exclusively?) used for equally spaced, noisy data
- ▶ Pros: easy, robust. Cons: converges slowly with N, expense of  $h_{\mu}(f_i)$
- Model's n-width (approximation properties) independent of data

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## Parameter estimation from "burst" signals

## GW model

$$h_{\mu}(t) = Ae^{-(t-t_c)^2/(2\alpha^2)} \sin(2\pi f_0(t-t_c)),$$

describes merging black holes or supernovae GW signals.

• 4 dimensional model  $\mu = (A, t_c, \alpha, f_0)$ 

#### Detector model

- Data segments of 32 second intervals
- Sampling rate of 64Hz such that observation every 1/64 seconds
- ► Frequency domain data samples (32 \* 64)/2
- White noise (set weight W = 1)
  - Same average amplitude  $|n(f_i)|$  at each frequency component  $f_i$

# Offline (data independent)

Decide on suitable range of parameters, run greedy algorithm



Left:  $(\alpha, f_0)$  points selected by the greedy algorithm. Right: Approximation error  $\|h_{\mu} - \mathcal{P}_n h_{\mu}\|^2$  as a function of greedy basis

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ROQ for parameterized inner products with noisy data

# Offline (data independent)

Identify ROQ nodes from empirical interpolation method



Left: EIM points  $\{F_i\}_{i=1}^{54}$  selected by the EIM algorithm. Right: Empirical interpolant approximation error  $\|h_{\mu_{c}} - \mathcal{I}_{\underline{n}}h_{\mu}\|_{=}^{2}$  and error bound

# Summary so far

- $\checkmark$  Greedy basis and ROQ points stored to file.
- $\checkmark$  Verified accuracy of basis and interpolation points.
- $\checkmark$  ROQ rule for this set of functions "Good for all time"

Some signal has been recorded!! Carry out parameter estimation...

# True signal parameters $\alpha = 1$ , $f_0 = 0.25$ , $t_c = 0.1$ , A unfixed Modeled noise

At each frequency  $n(f_i) = \mathcal{N}(0, \sigma^2)$ 

Mock data: Prepare data s = h + n, recover parameters with MCMC

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# Startup (data dependent)

Compute weights

$$\vec{\omega}^T = \vec{E}^T A^{-1}$$
  $E_j := \sum_{k=1}^N s^*(f_k) e_j(f_k) \Delta f$ 

where the  $j^{th}$  column of the matrix A is basis  $e_j$  evaluated at ROQ nodes



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Sample distribution  $p(\mu|s)$  where likelihood  $P(s|\mu)$  uses standard or ROQ

$$\langle s, h_{\mu} \rangle = \Delta f \sum_{i=1}^{N} s^{*}(f_{i}) h_{\mu}(f_{i}) \approx \sum_{i=1}^{n} \omega_{i} h_{\mu}(F_{i})$$



Left: Runtime. With 10<sup>8</sup> points standard  $\approx$  1day, ROQ  $\approx$  1 hour!! Right: Speed-up of MCMC algorithm using a standard and ROQ quadrature.

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		Recovered values			
SNR	R Method	$f_0$	α	$t_c$	A
5	Full	$0.217 \pm 0.069$	$0.896 \pm 0.194$	$0.068 \pm 0.104$	$1.704\pm0.379$
	ROQ	$0.217 \pm 0.068$	$0.897 \pm 0.196$	$0.069 \pm 0.104$	$1.702\pm0.375$
10	Full	$0.212 \pm 0.048$	$0.875 \pm 0.132$	$0.084 \pm 0.053$	$2.362\pm0.278$
	ROQ	$0.209 \pm 0.050$	$0.866 \pm 0.132$	$0.085\pm0.052$	$2.387 \pm 0.287$
20	Full	$0.225 \pm 0.029$	$0.891 \pm 0.093$	$0.092 \pm 0.028$	$2.944 \pm 0.176$
	ROQ	$0.224 \pm 0.029$	$0.892 \pm 0.093$	$0.093 \pm 0.028$	$2.944 \pm 0.177$
40	Full	$0.248 \pm 0.009$	$0.981 \pm 0.041$	$0.097 \pm 0.016$	$3.471 \pm 0.157$
	ROQ	$0.248 \pm 0.009$	$0.981 \pm 0.042$	$0.097 \pm 0.016$	$3.471 \pm 0.157$



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ROQ for parameterized inner products with noisy data

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#### Features

- Startup cost  $\approx$  time to compute inner products of data with basis (fast)
- Once weights specified, evaluations of  $\chi^2$  about 25 times faster
- Accuracy in recovered parameters is preserved

#### What about more complicated GW signals?



GW signal from two orbiting black holes ("chirp" signal)

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Two black holes of masses  $m_1$  and  $m_2$  rotate one another for long times

$$h_{\mu}(f) = \mathcal{A}f^{-7/6} \cdot \exp\left(i\left\{-\frac{\pi}{4} + \frac{3}{128}\left(\pi \cdot \frac{G}{c^3} \cdot f \cdot \mathcal{M}_c\right)^{-5/3}\right\} + \dots\right),$$

where  $\mu = \mathcal{M}_c = (m_1 m_2)^{3/5} (m_1 + m_2)^{-1/5}$ .

 $\mathcal{P} = [A,B]$  where  $A = 5 imes 10^{30}$  Kg and  $B = 50 imes 10^{30}$  Kg

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## Detector's noise curve

$$S(y) = 9 \times 10^{-46} \left[ (4.49y)^{-56} + 0.16y^{-4.52} + 0.52 + 0.32 \cdot y^2 \right], \quad y = \frac{f}{150 Hz}$$

is experimentally determined and implies a weight  $W = S^{-1}$ 

### Parameterized inner products

$$\int_{40}^{360} h_{\mu_1}^*(f) h_{\mu_2}(f) W(f) df$$

where  $\mu_1, \mu_2 \in \mathcal{P}$ 

## Building the ROQ

• Uses a two-step greedy approximate integrands  $h_{\mu_1}^*(f)h_{\mu_2}(f)W(f)$ 

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Inner product errors using i) Gauss-Legendre quadrature, ii) trapezoidal, iii) ROQ built from GQ, and iv) ROQ built from the trapezoidal



- Similar behavior between both ROQ rules (same basis)
- Only factor of 2 savings compared to GQ (predetermined points)
- Factor of 50 when using equally spaced "data" samples

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# Summary

- Introduced application/data specific quadrature for parameterized integrals
- Motivated by need to perform fast, accurate GW parameter estimation
- ▶ ROQ error decays like Kolmogorov *n*-width times a Lebesgue-like constant
- Offline costs high, online significantly faster

## Future work and open questions

- Implementation within existing GW analysis pipelines underway
- Uses as application specific nested quadrature rule?
- Better criteria to choose ROQ basis and points?
- Uses outside of data analysis?

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