Sparse grid quadrature as a knapsack problem

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Topics

- Weighted tensor product spaces
- Dimension adaptive sparse grid quadrature
- Lattice-constrained knapsack problems

An RKHS on $\mathcal{D}$ of functions with mean zero

Let $\mathcal{D} \subset \mathbb{R}^{s+1}$ be a compact s-dimensional manifold with probability measure μ, and let $\mathcal{H}$ be a reproducing kernel Hilbert space (RKHS) of functions $f : \mathcal{D} \to \mathbb{R}$, such that

$$\int_{\mathcal{D}} f(x)\, d\mu(x) = 0 \text{ for all } f \in \mathcal{H},$$

with kernel $\mathcal{K} : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$ such that for all $x \in \mathcal{D}$, the function k_x defined by $k_x(y) := \mathcal{K}(x, y)$ satisfies

$$k_x \in \mathcal{H}, \quad \text{and, for all } f \in \mathcal{H}, \quad \langle k_x, f \rangle_{\mathcal{H}} = f(x).$$

(Hickernell and Woźniakowski 2001; Sloan and Woźniakowski 2001; Kuo and Sloan, 2005)

The weighted space $\mathcal{H}^\gamma$

For $0 < \gamma \leqslant 1$, extend $\mathcal{H}$ into the space $\mathcal{H}^\gamma$ of all functions of the form

$$g = a\mathbf{1} + f,$$

where $\mathbf{1}(x) := 1$, $a \in \mathbb{R}$, and $f \in \mathcal{H}$, with norm

$$\|g\|^2_{\mathcal{H}^\gamma} := |a|^2 + \frac{1}{\gamma}\|f\|^2_{\mathcal{H}}.$$

$\mathcal{H}^\gamma$ is an RKHS with reproducing kernel

$$\mathcal{K}^\gamma(x, y) = 1 + \gamma\mathcal{K}(x, y),$$

where $\mathcal{K}$ is the reproducing kernel of $\mathcal{H}$.

(Hickernell and Woźniakowski 2001; Sloan and Woźniakowski 2001; Kuo and Sloan, 2005)

The weighted tensor product space $\mathcal{H}^{d,\gamma}$

Let $\gamma := (\gamma_1, \ldots, \gamma_d)$, with $1 \geqslant \gamma_1 \geqslant \ldots \geqslant \gamma_d > 0$.

On $\mathcal{D}^d$ define the tensor product RKHS

$$\mathcal{H}^{d,\gamma} := \bigotimes_{h=1}^{d} \mathcal{H}^{\gamma_h}.$$

The reproducing kernel of $\mathcal{H}^{d,\gamma}$ is

$$\mathcal{K}^{d,\gamma}(x, y) := \prod_{h=1}^{d} \mathcal{K}^{\gamma_h}(x_h, y_h).$$

(Hickernell and Woźniakowski 2001; Sloan and Woźniakowski 2001; Kuo and Sloan, 2005)

Quadrature rules on $\mathcal{H}^{d,\gamma}$

For $\{x_1, \ldots, x_n\} \subset \mathcal{D}^d$, the quadrature rule

$$Qf := \sum_{i=1}^{n} w_i f(x_i)$$

is a continuous linear functional on $\mathcal{H}^{d,\gamma}$, satisfying

$$Qf = \langle q, f \rangle_{\mathcal{H}^{d,\gamma}},$$

where

$$q := \sum_{i=1}^{n} w_i k_{x_i}^{d,\gamma}, \quad k_{x_i}^{d,\gamma}(y) := \mathcal{K}^{d,\gamma}(x_i, y).$$

(Wasilkowski and Woźniakowski 1999; Hickernell and Woźniakowski 2001)

Optimal quadrature weights on $\mathcal{H}^{d,\gamma}$

The worst case error

$$e(q) := \sup_{\|f\|_{\mathcal{H}^{d,\gamma}} \leqslant 1} \left| \int_{\mathcal{D}^d} f(x) d\mu_d(x) - \langle q, f \rangle_{\mathcal{H}^{d,\gamma}} \right|$$

satisfies

$$e(q)^2 = \|1 - q\|^2_{\mathcal{H}^{d,\gamma}} = \langle 1 - q, 1 - q \rangle_{\mathcal{H}^{d,\gamma}}$$

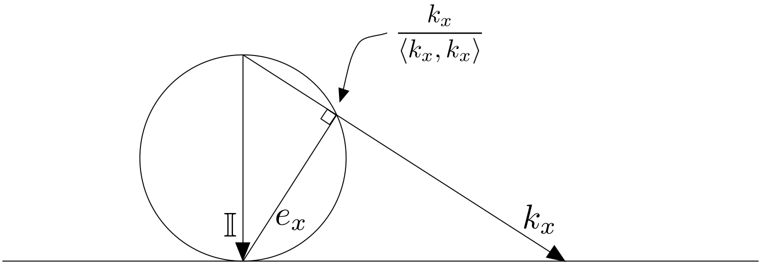
$$= 1 - 2 \sum_{i=1}^{n} w_i + w^T G w, \quad \text{where}$$

$$G_{i,j} := \langle k^{d,\gamma}_{x_i}, k^{d,\gamma}_{x_j} \rangle = \mathcal{K}^{d,\gamma}(x_i, x_j).$$

The weights w are optimal when $Gw = [1, \ldots, 1]^T$.

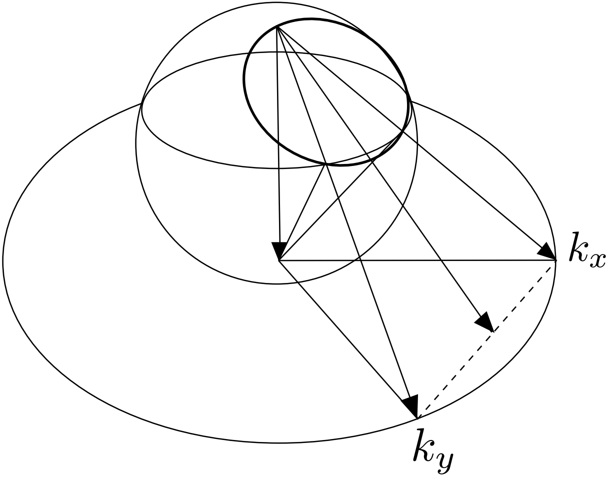
(Wasilkowski and Woźniakowski 1999)

Optimal weight for one quadrature point



(Illustration by Osborn, 2009)

Optimal weights for two quadrature points



(Illustration by Osborn, 2009)

Optimal quadrature in $\mathcal{H}^\gamma$

Consider a sequence of quadrature points $x_1, x_2, \ldots \in \mathcal{D}$, and a sequence of positive integers $m_0 < m_1 < \ldots$

For $j \geqslant 0$, let q_j^γ denote the optimal quadrature rule in

$$V_j^\gamma := \operatorname{span}\{k_{x_1}^\gamma, \ldots, k_{x_{m_j}}^\gamma\} \subset \mathcal{H}^\gamma.$$

Define the pair-wise orthogonal spaces U_j^γ by $U_0^\gamma = V_0^\gamma$, and by the orthogonal decomposition $V_{j+1}^\gamma = V_j^\gamma \oplus U_{j+1}^\gamma$.

Since the q_j^γ are optimal,

$$\delta_{j+1}^\gamma := q_{j+1}^\gamma - q_j^\gamma \in U_{j+1}^\gamma, \quad \text{and}$$
$$\delta_0^\gamma := q_0^\gamma \in U_0^\gamma = V_0^\gamma.$$

(Gerstner and Griebel 1998; Wasilkowski and Woźniakowski 1999)

Multi-indices and down-sets

Elements of $\mathbb{J} := \mathbb{N}^d$ are treated as multi-indices, with a partial order such that for $i, j \in \mathbb{J}$, $i \leqslant j$ if and only if $i_h \leqslant j_h$ for all h from 1 to d.

For a multi-index $i \in \mathbb{J}$, let $\downarrow i$ denote the down-set of i, defined by $\downarrow i := \{j \in \mathbb{J} \mid j \leqslant i\}$.

Subsets of $\mathbb{J}$ are partially ordered by set inclusion.
For a subset $X \subset \mathbb{J}$, let $\downarrow X$ denote the down-set of X, defined by $\downarrow X := \bigcup_{i \in X} \downarrow i$.

Then $\downarrow X$ is the smallest set $Y \supseteq X$ such that if $i \in Y$ and $j \leqslant i$ then $j \in Y$. Thus $\downarrow\downarrow X = \downarrow X$.

(Davey and Priestley 1990)

Sparse grid quadrature in $\mathcal{H}^{d,\gamma}$

A sparse grid quadrature rule in $\mathcal{H}^{d,\gamma}$ is of the form

$$q \in V_I := \sum_{j \in I} \bigotimes_{h=1}^{d} V_{j_h}^{\gamma_h}$$

for some index set $I \subset \mathbb{J} = \mathbb{N}^d$.

(Gerstner and Griebel 1998; Wasilkowski and Woźniakowski 1999)

Sparse grid quadrature in $\mathcal{H}^{d,\gamma}$ (cont.)

From the orthogonal decomposition $V_j^\gamma = \bigoplus_{i=1}^{j} U_i^\gamma$
one derives the multidimensional orthogonal decomposition

$$V_I = \bigoplus_{j \in \downarrow I} \bigotimes_{h=1}^{d} U_{j_h}^{\gamma_h},$$

An optimal $q \in V_I$ is obtained as

$$q_I = \sum_{j \in \downarrow I} \bigotimes_{h=1}^{d} \delta_{j_h}^{\gamma_h}.$$

Thus both V_I and q_I are obtained in terms of the down-set $\downarrow I$, effectively restricting our choice of the set I to down-sets.

(Gerstner and Griebel 1998; Hegland 2003)

A dimension adaptive algorithm to choose I

Here, $m^{(h)}_{j_h} := \dim U^{\gamma_h}_{j_h}$, $\delta^{(h)}_{j_h} := \delta^{\gamma_h}_{j_h}$,
$n_j := \prod_{h=1}^{d} m^{(h)}_{j_h}$, $\Delta_j := \bigotimes_{h=1}^{d} \delta^{(h)}_{j_h}$.

Algorithm 1: A dimension adaptive algorithm.

Data: accuracy ϵ, incremental rules Δ_j and costs n_j for $j \in \mathbb{J}$
Result: ϵ approximation q and index set I
$I := \{0\};\quad q := \Delta_0$;
while $\|1 - q\| > \epsilon$ **do**
  $i := \operatorname{argmax}_j \{\|\Delta_j\|^2 / n_j \mid I \cup \{j\}$ is a down-set$\}$;
  $I := I \cup \{i\};\quad q := q + \Delta_i$;

(Hegland 2003; Gerstner and Griebel 2003)

Our optimization problem

Our optimization problem is to maximize

$$p(X) := \sum_{i \in X} p_i,$$

subject to

$$n(\downarrow X) := \sum_{i \in \downarrow X} n_i \leqslant N, \qquad (1)$$

where $p_i := \|\Delta_i\|^2 \in \mathbb{R}_+$ and n_i and N are in $\mathbb{N}_+$, that is, the p_i are positive real numbers and the n_i and N are positive integers.

(Gerstner and Griebel 1998; Hegland 2003; Gerstner and Griebel 2003)

The admissibility condition of problem (1)

The solution of the optimisation problem (1) satisfies an admissibility condition:

Proposition 1

If $\boldsymbol{X}$ *is a solution of the optimisation problem* (1) *then*

$$\boldsymbol{X} = \downarrow \boldsymbol{X}. \tag{2}$$

(Gerstner and Griebel 1998; Hegland 2003; Gerstner and Griebel 2003)

The related classical knapsack problem

A widely studied problem in optimisation is the knapsack problem. The knapsack problem related to our problem (1) is to maximize

$$p(X) = \sum_{i \in X} p_i,$$

subject to

$$n(X) = \sum_{i \in X} n_i \leqslant N, \tag{3}$$

where $p_i \in \mathbb{R}_+$ and n_i and N are in $\mathbb{N}$.

(Dantzig 1957)

A lattice-constrained knapsack problem

We can now formulate a converse of Proposition 1.

Proposition 2

If $\boldsymbol{X}$ *is a solution of the knapsack problem* (3), *and satisfies the admissibility condition* $\boldsymbol{X} = \downarrow \boldsymbol{X}$, *then it is a solution of the optimization problem* (1).

This justifies our calling problem (1) a lattice-constrained knapsack problem.

Monotonicity

One says that $\boldsymbol{p} \in \mathbb{R}_+^{\mathbb{J}}$ is monotonically decreasing if $\boldsymbol{i} < \boldsymbol{j}$ implies that $\boldsymbol{p_i} \geqslant \boldsymbol{p_j}$.

If $\boldsymbol{i} < \boldsymbol{j}$ implies that $\boldsymbol{p_i} > \boldsymbol{p_j}$, one says that $\boldsymbol{p} \in \mathbb{R}_+^{\mathbb{J}}$ is strictly decreasing.

The definitions of “monotonically increasing” and “strictly increasing” are similar.

Monotonicity implies admissibility

The following proposition holds.

Proposition 3

If $\boldsymbol{p} \in \mathbb{R}_+^{\mathbb{J}}$ *is monotonically decreasing and* $\boldsymbol{n} \in \mathbb{N}_+^{\mathbb{J}}$ *is monotonically increasing, there exists a solution of the knapsack problem* (3) *which also solves the optimization problem* (1).

If $\boldsymbol{p}$ *is strictly decreasing, then any solution of* (3) *is a solution of* (1).

One can therefore use any method to solve the knapsack problem (3), check admissibility (2), and then swap multi-indices to get a solution of problem (1).

Enumeration by decreasing efficiency

The algorithm we adapt is based on efficiency $r_i := p_i/n_i$, and generates the initial values of an enumeration $i^{(t)}$ of $\mathbb{J}$, $t \in \mathbb{N}_+$, satisfying

$$r_{i^{(t)}} \geqslant r_{i^{(t+1)}}.$$

The algorithm recursively generates $i^{(t+1)}$ from $i^{(t)}$, until for some T the condition

$$n(X_{(T)}) \leqslant N < n(X_{(T+1)})$$

holds, where

$$X_{(t)} := \bigcup_{s=1}^{t} i^{(s)}.$$

(Dantzig 1957; Bungartz and Griebel 1999)

Enumeration by decreasing efficiency (cont.)

One then gets

Proposition 4

The construction of $\boldsymbol{i}^{(t)}$ *terminates for some* $t = T$.

Also, if $\boldsymbol{p}$ *is strictly decreasing,* $\boldsymbol{n}$ *is monotonically increasing, and* $\boldsymbol{n}(\boldsymbol{X}_{(T)}) = \boldsymbol{N}$, *then* $\boldsymbol{X}_{(T)}$ *is a solution of problem* (1).

(Dantzig 1957; Bungartz and Griebel 1999)

Finite construction

The construction of the enumeration requires sorting an infinite sequence and is thus not feasible in general, but, in the case where $\boldsymbol{p}$ is monotonically decreasing and $\boldsymbol{n}$ is monotonically increasing, the enumeration can be done recursively in finite time.

In this case $\boldsymbol{r}$ is monotonically decreasing. By construction, $\boldsymbol{r}_{\boldsymbol{i}^{(t)}} \geqslant \boldsymbol{r}_{\boldsymbol{i}^{(t+1)}}$, so the enumeration cannot have $\boldsymbol{i}^{(t)} \geqslant \boldsymbol{i}^{(t+1)}$.

It follows that $\boldsymbol{i}^{(1)} = \mathbf{0}$.

(Hegland 2003; Gerstner and Griebel 2003)

Minimal elements

The element $\boldsymbol{i}$ is a minimal element of a subset of $\mathbb{J}$ if there are no elements $\boldsymbol{j} < \boldsymbol{i}$ in that subset. The minimum is thus with respect to the lattice defined by the partial order in $\mathbb{J}$.

Since $\boldsymbol{i}^{(t)}$ is an enumeration of $\mathbb{J}$, no element occurs twice, and so $\boldsymbol{i}^{(t+1)} \in \boldsymbol{X}^{C}_{(t)} := \mathbb{J} \setminus \boldsymbol{X}_{(t)}$.

Any later element $\boldsymbol{i}^{(t+1+s)}$ in the enumeration cannot be smaller than $\boldsymbol{i}^{(t+1)}$, so $\boldsymbol{i}^{(t+1)}$ is a minimal element of $\boldsymbol{X}^{C}_{(t)}$.

The set $\boldsymbol{M}_{(t)}$ of minimal elements of $\boldsymbol{X}^{C}_{(t)}$ is finite.
One can thus find $\boldsymbol{j} = \boldsymbol{i}^{(t+1)}$ with largest $\boldsymbol{r}_{\boldsymbol{j}}$ in this set.

(Hegland 2003; Gerstner and Griebel 2003)

Construction of set of minimal elements $M_{(t)}$

To construct the set of minimal elements of $X^C_{(t)}$, we define $S(i)$, the forward neighbourhood of $i \in \mathbb{J}$, as

$$S(i) := \{j \in \mathbb{J} \mid i < j \text{ and } (i \leqslant \ell < j \Rightarrow \ell = i)\},$$

that is, $S(i)$ is the set of minimal elements of $\{j \in \mathbb{J} \mid i < j\}$.

Let e be the standard basis of $\mathbb{R}^{\mathbb{J}}$.

To construct $M_{(t)}$, start with
$M_{(1)} = S(i^{(1)}) = S(0) = \{e_1, \ldots, e_d\}$.

Then given $M_{(t-1)}$ and $i^{(t)}$, obtain
$M_{(t)} = \left(M_{(t-1)} \setminus \{i^{(t)}\}\right) \cup S(i^{(t)})$.

(Hegland 2003; Gerstner and Griebel 2003)

Review of the dimension adaptive algorithm

Algorithm 2: A dimension adaptive algorithm.

Data: accuracy ϵ, incremental rules $\boldsymbol{\Delta}_j$ and costs n_j for $j \in \mathbb{J}$
Result: ϵ approximation q and index set I
$I := \{0\}; \quad q := \boldsymbol{\Delta}_0$;
while $\|1 - q\| > \epsilon$ **do**
  $i := \operatorname{argmax}_j \{\|\boldsymbol{\Delta}_j\|^2 / n_j \mid I \cup \{j\}$ is a down-set$\}$;
  $I := I \cup \{i\}; \quad q := q + \boldsymbol{\Delta}_i$;