A quasi-Monte Carlo data compression algorithm for machine learning

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Quasi-Monte Carlo for PDEs

- More than 100 years of QMC

  [Weyl 1916], [Koksma 1942], [Hlawka 1962], [Sobol 1967], [Niederreiter 1988], [Faure 1982],...

$$-\mathrm{div}(A(\boldsymbol{y})\nabla u(x,\boldsymbol{y})) = f(x) \quad \text{compute} \quad \int_{[0,1]^s} G(u(\cdot,\boldsymbol{y}))\,d\boldsymbol{y}$$

- QMC for parametric equations
  - [Graham, Kuo, Nuyens, Scheichl, Sloan 2011]
  - [Dick, Kuo, Le Gia, Nuyens, Schwab 2015]
  - [Graham, Kuo, Nichols, Scheichl, Schwab, Sloan 2015]

- Higher-order QMC for random PDEs
  - [Dick, Kuo, Le Gia, Nuyens, Schwab 2014]

Improvement: $\mathcal{O}(N^{-1/2}) \longrightarrow \mathcal{O}(N^{-1+\delta}) \longrightarrow \mathcal{O}(N^{-\alpha})$

Neural Networks

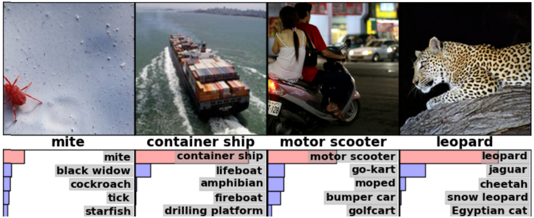
Parametrized set of functions $f(x, \mathcal{W})$

- $x \in \mathbb{R}^n \ldots$ input, $\mathcal{W} \in \mathbb{R}^N \ldots$ weights

Feedforward networks

$$f(x, \mathcal{W}) = W_d \phi(W_{d-1} \phi(\ldots \phi(W_0 x + b_0) \ldots)) + b_d$$

- Image classification (AlexNet, 2012)



- Speech recognition (transformers 2017, long-term-short-term networks 1997)

Machine learning in numerical analysis

Deep Ritz method [E-Yu, 2018]

- Solving the PDE

$$-\Delta u = f \quad \text{with b.c.} \quad u = 0$$

- equivalent to minimizing

$$\min_{u \in H_0^1(D)} \frac{1}{2} \|\nabla u\|_{L^2(D)}^2 - \langle f \, , \, u \rangle_{L^2(\Omega)}$$

Use NN to parametrize $u(x) = u(x, \mathcal{W})$, minimize [Fu-Wang 2021 $\rightarrow$ QMC]

$$\min_{\mathcal{W}} \frac{1}{N} \sum_{i=1}^{N} |\nabla u|^2(x_i) - 2f(x_i)u(x_i)$$

Machine learning in numerical analysis

Weak Adversarial Networks [Zang et al., 2019]

- Solving the PDE

$$\langle \nabla u\,,\,\nabla v\rangle_{L^2(D)} = \langle f\,,\,v\rangle_{L^2(D)} \quad \text{for all } v \in H^1_0(D)$$

- solve min-max problem

$$\min_{u\in H^1_0(D)} \max_{v\in H^1_0(D)} \left|\langle \nabla u\,,\,\nabla v\rangle_{L^2(D)} - \langle f\,,\,v\rangle_{L^2(D)}\right|^2$$

Use NN to parametrize $u(x) = u(x, \mathcal{W})$ and $v(x) = v(x, \mathcal{W}')$

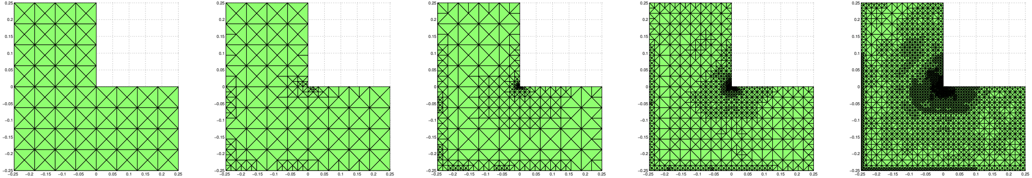
$$\min_{\mathcal{W}} \max_{\mathcal{W}'} \left|\frac{1}{N}\sum_{i=1}^{N} \nabla u(x_i)\nabla v(x_i) - f(x_i)v(x_i)\right|^2$$

Machine learning for adaptive mesh refinement

- Galerkin method: find $U_\ell \in \mathcal{X}_\ell$ s.t.

$$\langle \nabla U_\ell \,,\, \nabla V \rangle = \langle f \,,\, V \rangle \quad \text{for all } V \in \mathcal{X}_\ell$$

$$\boxed{\text{compute } U_\ell} \longrightarrow \boxed{\text{estimate } \rho_\ell} \longrightarrow \boxed{\text{mark}} \longrightarrow \boxed{\text{refine}}$$



Optimal adaptivity

Question: how to obtain optimal sequence $\mathcal{X}_\ell$

$$\|u - U_\ell\| \leq C(\dim \mathcal{X}_\ell)^{-s}$$

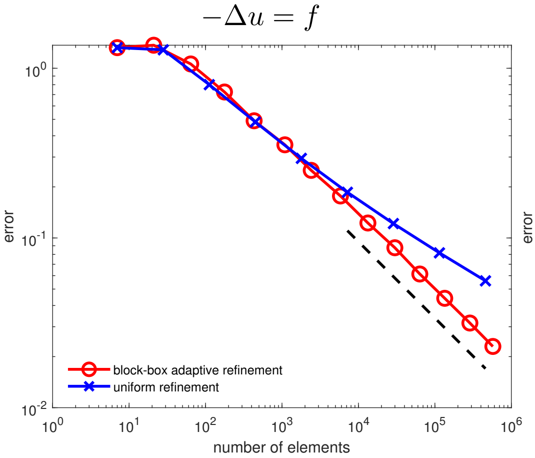
- Traditional adaptive algorithms are problem dependent
- Remedy: black-box algorithms with recurrent neural networks

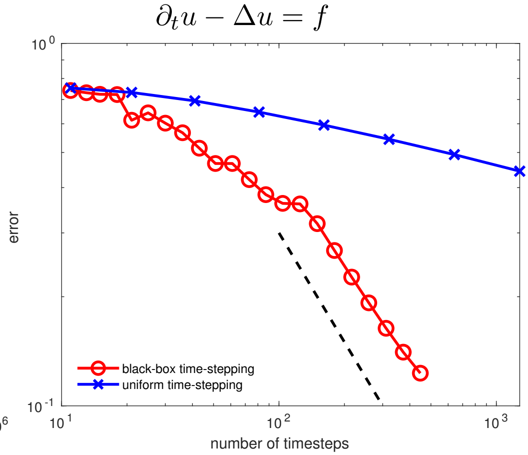
Theorem [Bohn-F. 2019]

The deep RNN $\mathrm{ADAPTIVE}$ is (almost) optimal with high probability, i.e.

$$\sup_{\substack{\ell\in\mathbb{N}\\ \|u-U_\ell\|\geq\varepsilon_{\mathrm{tol}}}} \|u - U_\ell\| N_\ell^s \leq C$$

Beats non-adaptive methods





Success at high cost

- Electronic Schrödinger equation [Gerard, Scherbela, Marquetand, Grohs 2021]
  - 50-100k epochs
- High dimensional Black-Scholes equation [Grohs, Hornung, Jentzen, Wurstemberger 2018]
- Weak GAN
  - 20k epochs for error $\approx 10^{-2}$
- AlexNet
  - 90 epchos with 1.2 million images

$\Longrightarrow$ Need for efficient training methods

Data fitting

- data $X = \{x_1, \dots, x_N\} \subset [0,1]^s$
- responses $Y = \{y_1, \dots, y_N\} \subset \mathbb{R}$

Aim: Find a predictor

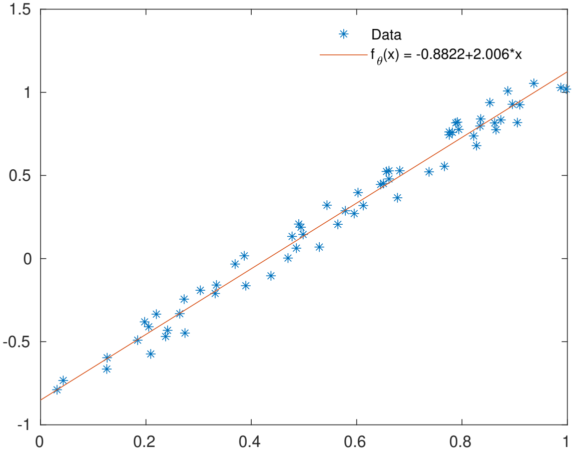
$$f_{\mathcal{W}} : [0,1]^s \to \mathbb{R}, \quad f_{\mathcal{W}}(x_i) \approx y_i, \quad i = 1, 2, \dots, N$$

Example:

$$f_{\mathcal{W}}(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_s x_s, \quad \mathcal{W} = (\beta_0, \beta_1, \dots, \beta_s);$$

Example: $f_{\mathcal{W}}$ is Neural Network

Data fitting



Training

Quality of predictor:

$$\begin{aligned}\mathrm{err}_{X,y}(f_{\mathcal{W}}) &= \frac{1}{N}\sum_{n=1}^{N}(f_{\mathcal{W}}(x_n) - y_n)^2 + R_{\mathcal{W}} \\ &= \frac{1}{N}\sum_{n=1}^{N} f_{\mathcal{W}}^2(x_n) - \frac{2}{N}\sum_{n=1}^{N} y_n f_{\mathcal{W}}(x_n) + \frac{1}{N}\sum_{n=1}^{N} y_n^2 + R_{\mathcal{W}}\end{aligned}$$

- choose the parameters $\mathcal{W}$ such that $\mathrm{err}_{X,y}(f_{\mathcal{W}})$ is 'small'.
- many evaluations of $\mathrm{err}_{X,y}(f_{\mathcal{W}})$ might be required
- Lasso (least squares with ℓ_1-constraint), gradient descent

Cost reduction techniques

Gradient descent requires to compute

$$\frac{1}{N}\sum_{n=1}^{N}\nabla_{\mathcal{W}}(f_{\mathcal{W}}(x_n)-y_n)^2$$

- Batch gradient descent: compute random sample of $M \ll N$ terms of sum

$$\frac{1}{N}\sum_{n=1}^{N}\nabla_{\mathcal{W}}(f_{\mathcal{W}}(x_n)-y_n)^2 \approx \frac{1}{M}\sum_{k=1}^{M}\nabla_{\mathcal{W}}(f_{\mathcal{W}}(x_{n_k})-y_{n_k})^2$$

- Support points [Mak-Joseph 2018]: target distribution Y

$$\arg\min_{z_1,\ldots,z_M}\Big\{\frac{2}{M}\sum_{i=1}^{M}\mathbb{E}\|z_i-Y\| - \frac{1}{M^2}\sum_{i,j=1}^{M}\|z_i-z_j\|\Big\}$$

- Sketching algorithms, see e.g. [Ahfock, Astle 2017]

Idea

Find an approximation of $\mathrm{err}_{X,y}(f_{\mathcal{W}})$ which can be computed in less than N operations.

We need to approximate two terms:

$$\frac{1}{N}\sum_{n=1}^{N} f_{\mathcal{W}}^2(x_n)$$

and

$$\frac{1}{N}\sum_{n=1}^{N} y_n f_{\mathcal{W}}(x_n).$$

Idea

Let $P = \{z_1, \dots, z_M\} \subset [0,1]^s$ be a set of points with $M \ll N$

- calculate weights $(W_{X,P}(z_m))_{1 \leq m \leq M}$ such that

$$\frac{1}{N} \sum_{n=1}^{N} f_{\mathcal{W}}^2(x_n) \approx \sum_{m=1}^{M} f_{\mathcal{W}}^2(z_m) W_{X,P}(z_m)$$

- weights $(W_{X,y,P}(z_m))_{1 \leq m \leq M}$ such that

$$\frac{1}{N} \sum_{n=1}^{N} y_n f_{\mathcal{W}}(x_n) \approx \sum_{m=1}^{M} f_{\mathcal{W}}(z_m) W_{X,y,P}(z_m)$$

Decoupling training from data

We then find 'optimal' parameters $\mathcal{W}$ by minimizing

$$\sum_{m=1}^{M} f_{\mathcal{W}}^2(z_m) W_{X,P}(z_m) - 2 \sum_{m=1}^{M} f_{\mathcal{W}}(z_m) W_{X,y,P}(z_m) + \frac{1}{N} \sum_{n=1}^{N} y_n^2 + R_{\mathcal{W}}$$

- Computing the weights $W_{X,P}(z_m)$ and $W_{X,y,P}(z_m)$ depends on N and M, but not on $\mathcal{W}$.
- Finding 'optimal' $\mathcal{W}$ depends on M and the number of optimization steps, but not on N.

$$\#\text{opt.steps} + \#\text{data} \ll \#\text{opt.steps} \times \#\text{data}$$

Digital Nets

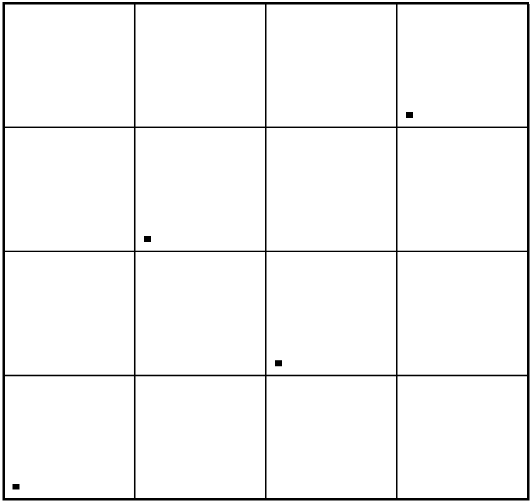
$P = \{z_1, \ldots, z_M\}$ is a (t, m, s) net in base b $(M = b^m)$

- Elementary interval in base b:

$$I_{\boldsymbol{a},\boldsymbol{d},m} = \prod_{j=1}^{s} \left[\frac{a_j}{b^{d_j}}, \frac{a_j + 1}{b^{d_j}}\right), d_1 + \cdots + d_s = m - t, 0 \leq a_j < b^{d_j}$$

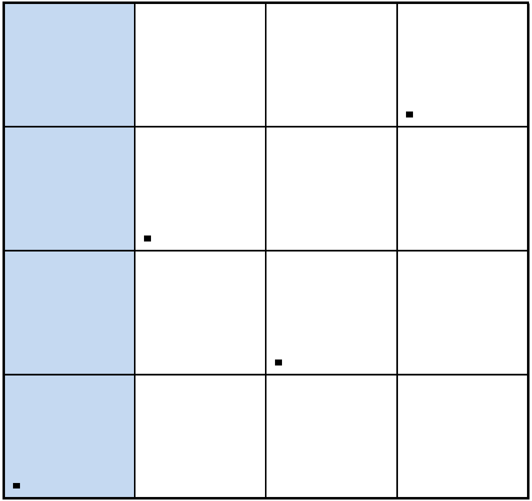
- For fixed $\boldsymbol{d} = (d_1, \ldots, d_s)^\top$ we get a partition of $[0,1)^s$ as $\boldsymbol{a} = (a_1, \ldots, a_s)^\top$ runs through all admissible choices.
- $\mathrm{Vol}(I_{\boldsymbol{a},\boldsymbol{d}}) = b^{t-m}$
- P is a (t, m, s)-net if each elementary interval contains exactly b^t points.

Digital net



The shaded region contains exactly one point.

Digital net



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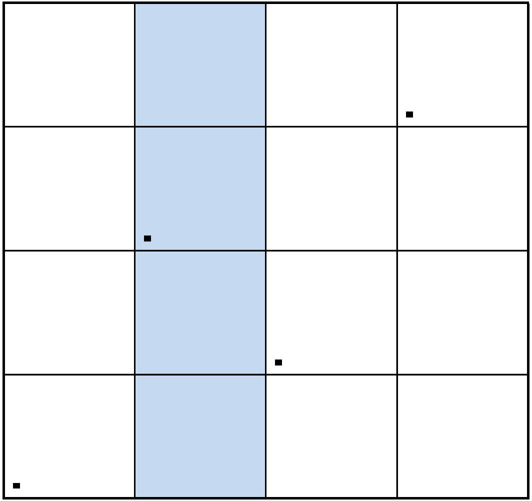

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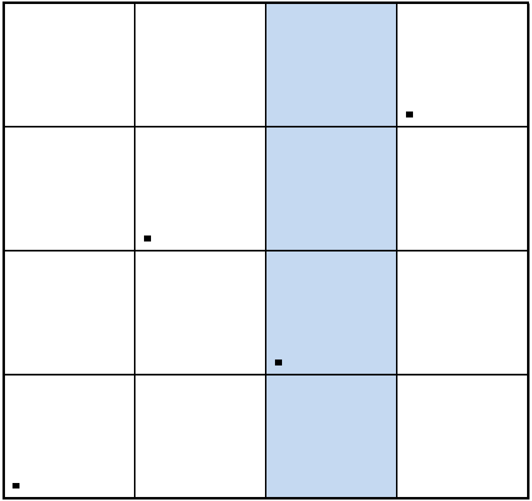
Digital net



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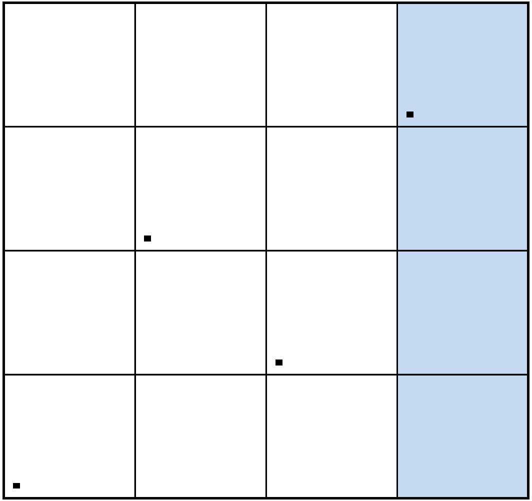
Digital net



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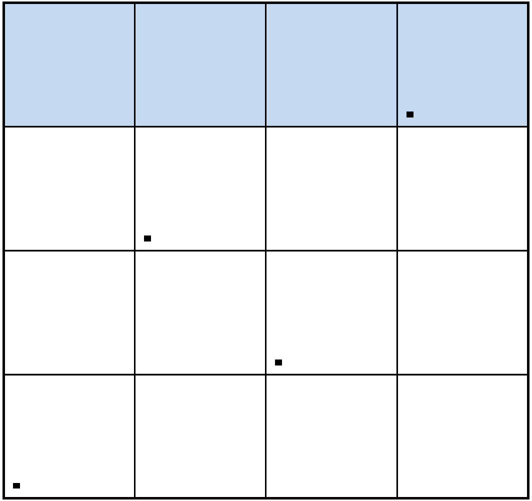
Digital net



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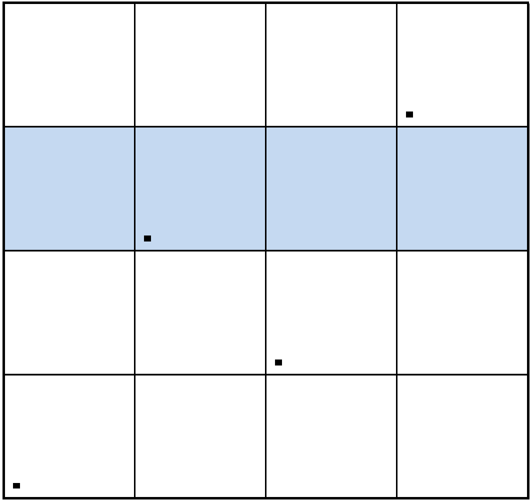
Digital net



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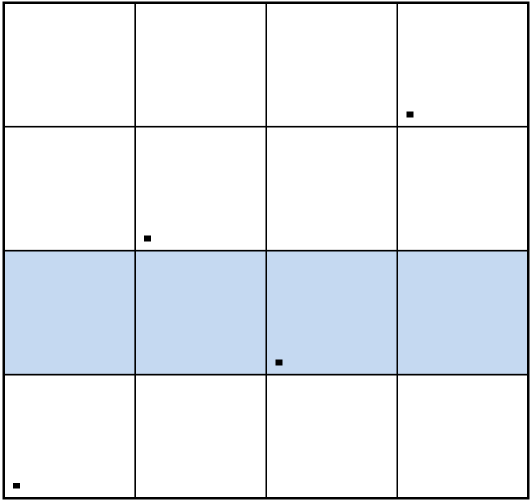

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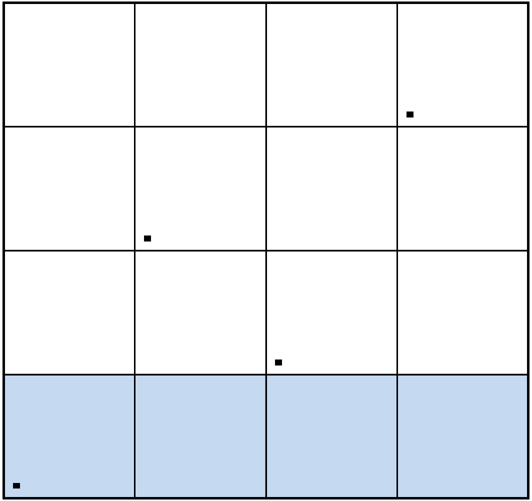
Digital net



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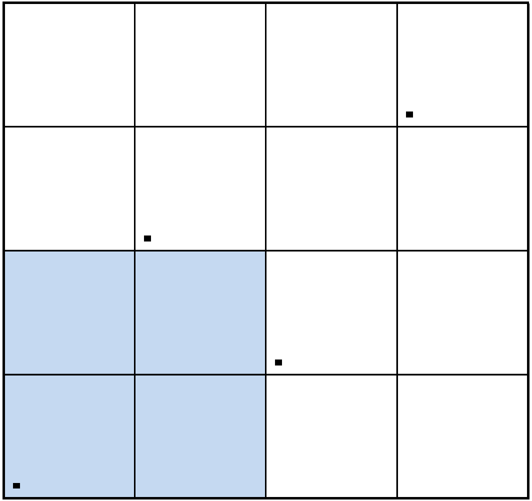
Digital net



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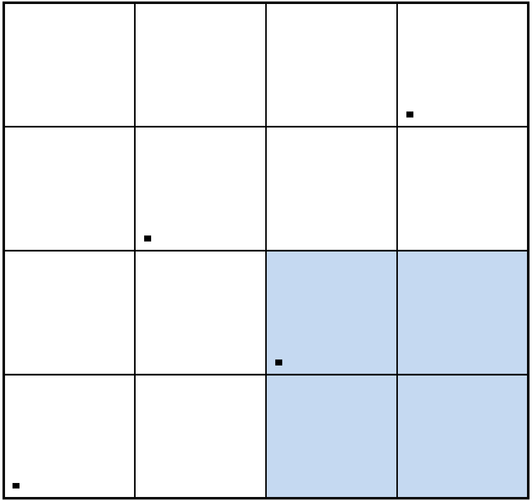

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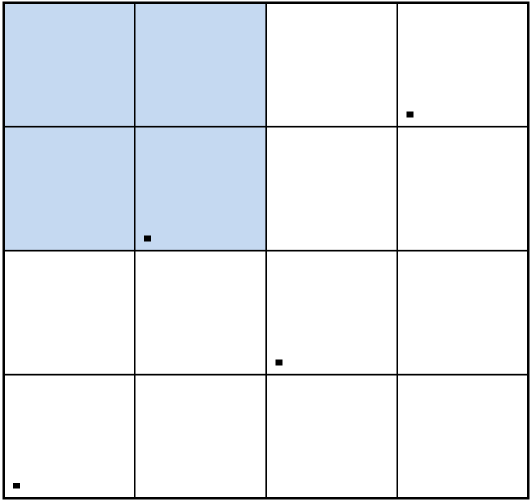
Digital net



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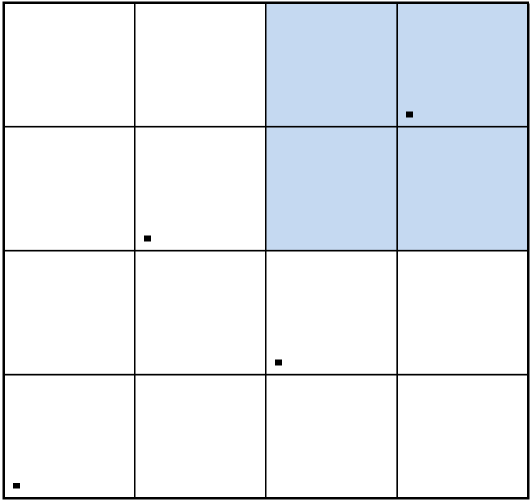
Digital net



The shaded region contains exactly one point.

Digital net constructions

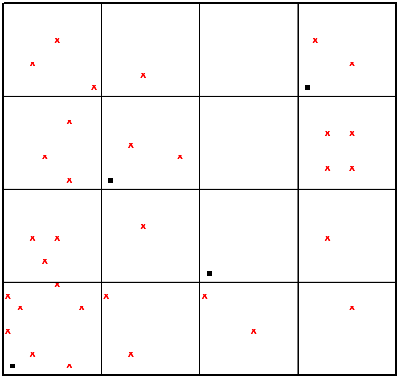
- Choose generator matrices $C_1, \dots, C_s$
- define i-th coordinate of digital net point z_m by

$$z_{m,i} = c_1 b^{-1} + c_2 b^{-2} + \dots \quad \text{where} \quad \boldsymbol{c} = C^i \boldsymbol{m} \text{ in } \mathbb{F}_b$$

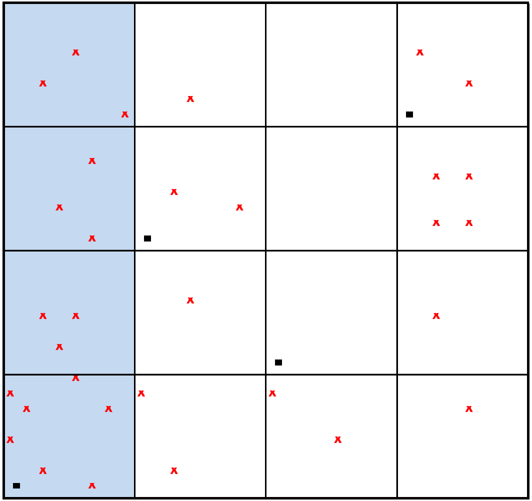
  with $m = m_0 + m_1 b + m_2 b^2 + \dots$
- Sobol' sequence (1967)
- Niederreiter sequences (1988) based on polynomials in $\mathbb{F}_b$
- t-value optimized Sobol' sequences [Joe-Kuo 2008]

How should we choose the weights $W_{X,P}(z_m)$?

Given: Digital net P (black) and data points X (red).

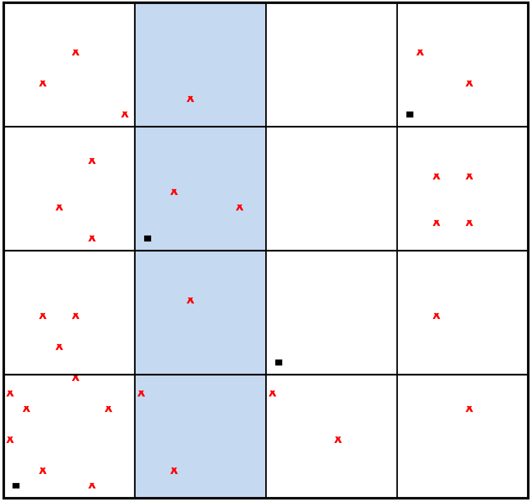


How should we choose the weights $W_{X,P}(z_m)$?



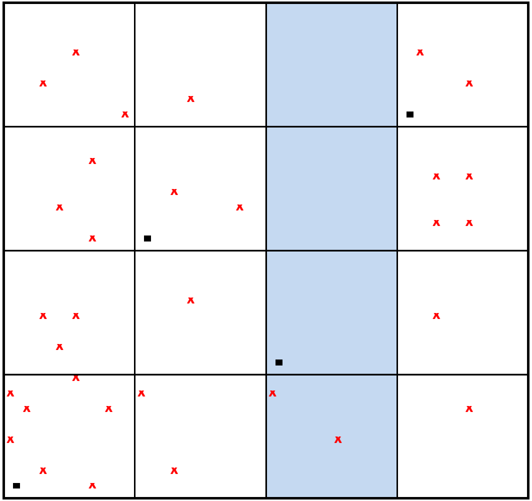
The shaded region contains 16 out of 32 data points

How should we choose the weights $W_{X,P}(z_m)$?



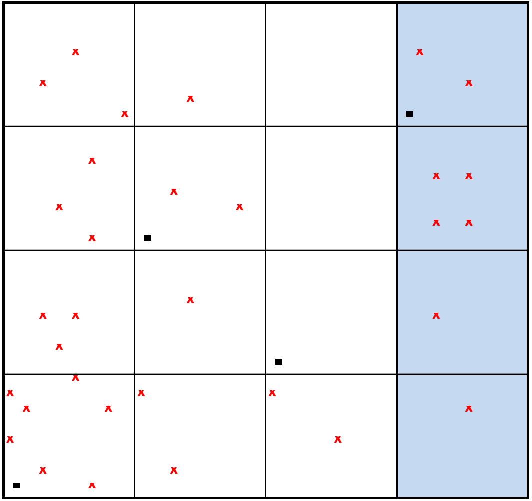
The shaded region contains 6 out of 32 data points

How should we choose the weights $W_{X,P}(z_m)$?



The shaded region contains 2 out of 32 data points

How should we choose the weights $W_{X,P}(z_m)$?



The shaded region contains 8 out of 32 data points

How should we choose the weights $W_{X,P}(z_m)$?

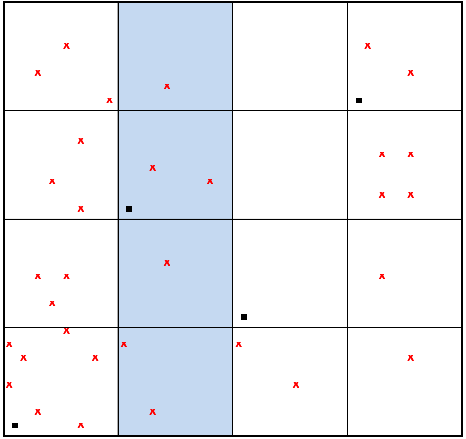
So the weights based on this partition should be

$$
\begin{aligned}
W_{X,P}(z_1) &= \frac{16}{32} = \frac{1}{2}, \\
W_{X,P}(z_2) &= \frac{6}{32} = \frac{3}{16}, \\
W_{X,P}(z_3) &= \frac{2}{32} = \frac{1}{16}, \\
W_{X,P}(z_4) &= \frac{8}{32} = \frac{1}{4};
\end{aligned}
$$

$\Rightarrow$ We can also use all the other possible partition into elementary intervals simulatenously.

Average data density

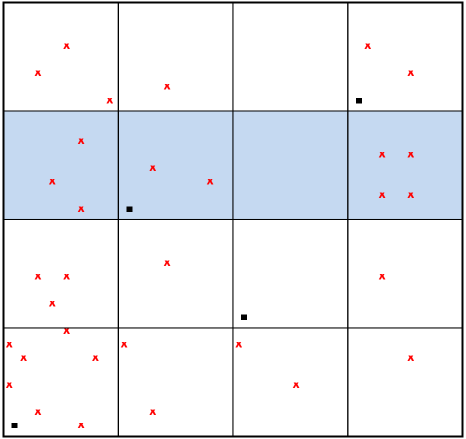
"How many data points can be reached from z_m with elementary interval of volume $2^{-\ell}$"



The shaded region contains 6 out of 32 data points

Average data density

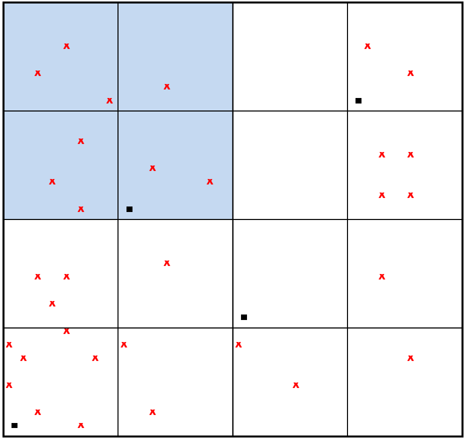
"How many data points can be reached from z_m with elementary interval of volume $2^{-\ell}$"



The shaded region contains 9 out of 32 data points

Average data density

“How many data points can be reached from z_m with elementary interval of volume $2^{-\ell}$”



The shaded region contains 9 out of 32 data points

Final result

The formula for $W_{X,P}(z_m)$ using all possible partitions is

$$\sum_{q=0}^{s-1}(-1)^q\binom{s-1}{q}\frac{b^{-(m'-m)-q}}{N}\sum_{\substack{\boldsymbol{d}\in\mathbb{N}_0^s\\|\boldsymbol{d}|=m-q}}\sum_{\substack{\boldsymbol{a}\in K_{\boldsymbol{d}}\\z_m\in I_{\boldsymbol{a},\boldsymbol{d}}}}\#(\mathcal{X}\cap I_{\boldsymbol{a},\boldsymbol{d},m}).$$

We use the approximation

$$\frac{1}{N}\sum_{n=1}^{N}f(x_n)^2\approx M_{m,m'}(f,\mathcal{X})=\sum_{\ell=1}^{b^{m'}}f(z_\ell)^2W_{\mathcal{X},P}(z_\ell).$$

Efficient computation

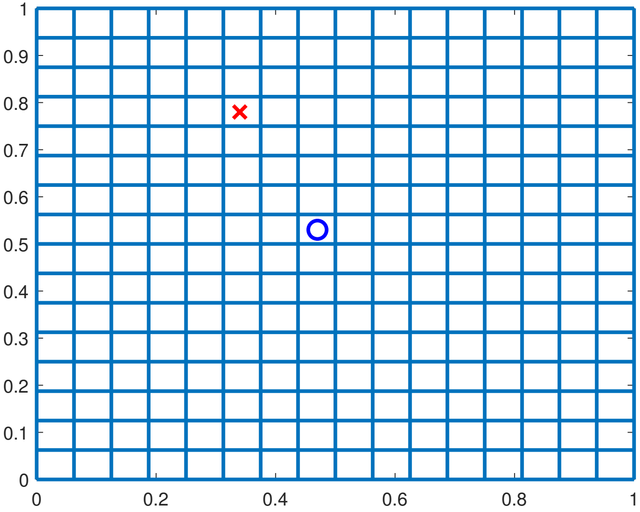
Main challenge is to compute

$$S_\ell(z_m) := \sum_{\substack{\boldsymbol{d}\in\mathbb{N}_0^s \\ |\boldsymbol{d}|=\ell}} \sum_{\substack{\boldsymbol{a}\in K_{\boldsymbol{d}} \\ z_m\in I_{\boldsymbol{a},\boldsymbol{d}}}} \#(\mathcal{X}\cap I_{\boldsymbol{a},\boldsymbol{d}})$$

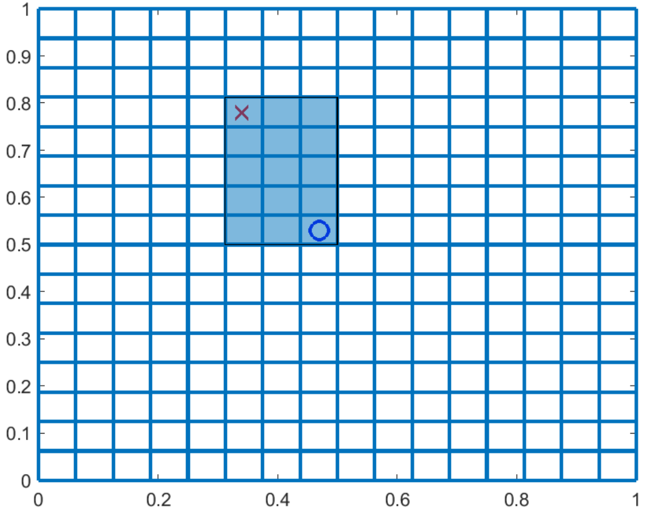
- $b^\ell\binom{\ell+s-1}{s-1}$ elementary intervals
- direct computation intractable

$\Longrightarrow$ Use properties of dyadic intervals

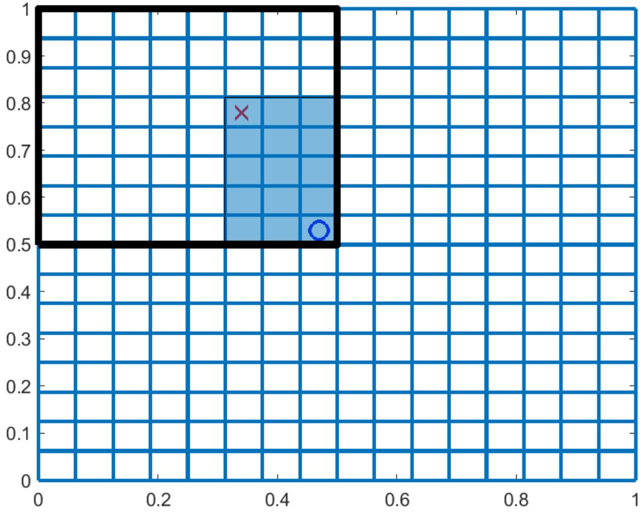
Efficient computation



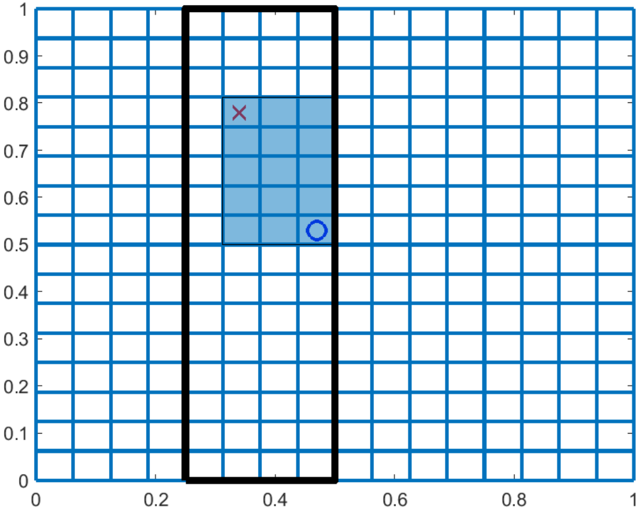
Efficient computation



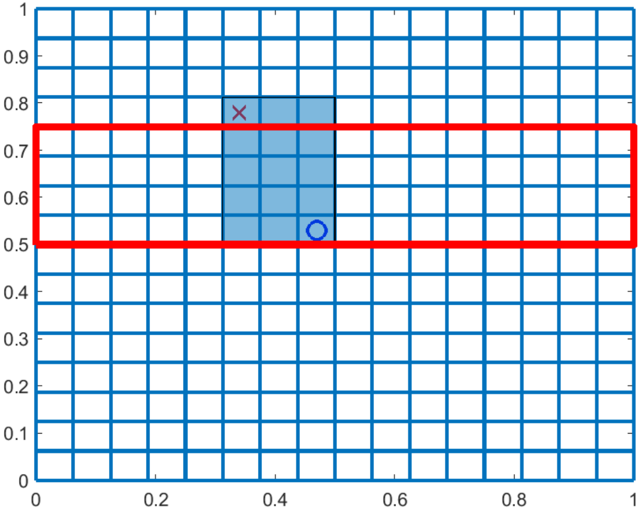
Efficient computation



Efficient computation



Efficient computation



Efficient computation

Given data point x and net point z_m

- for each dimension $j = 1, \ldots, s$
  - find largest $i_j \in \mathbb{N}$ with

$$ab^{-i_j} \leq x_j, z_{m,j} < (a+1)b^{-i_j} \quad \text{for some } a \in \mathbb{N}$$

- use equivalence

$$\#\big\{I_{\boldsymbol{a},\boldsymbol{d}} \,:\, z_m, x \in I_{\boldsymbol{a},\boldsymbol{d}}, |I_{\boldsymbol{a},\boldsymbol{d}}| = b^{-\ell}\big\} = \#\big\{\boldsymbol{d} \in \mathbb{N}^s \,:\, |\boldsymbol{d}| = \ell, \boldsymbol{d} \leq \boldsymbol{i}\big\}$$

- sum over all data points $x \in \mathcal{X}$

Efficient computation

Remains to compute

$$N(\ell,s,\boldsymbol{i}) = \#\{\boldsymbol{d}\in\mathbb{N}^s \,:\, |\boldsymbol{d}|=\ell, \boldsymbol{d}\le\boldsymbol{i}\}$$

Use recursion

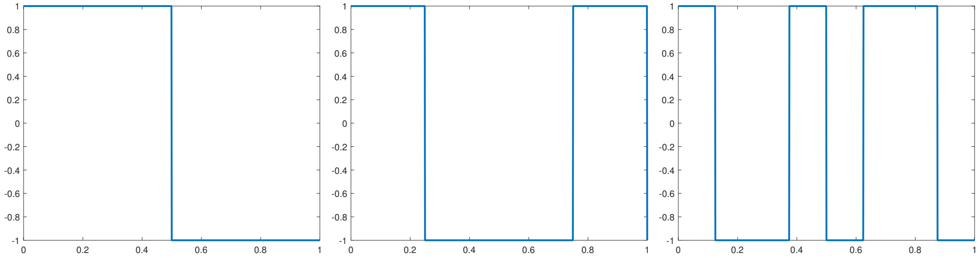
$$N(\ell,s,\boldsymbol{i}) = \sum_{k=\ell-i_s}^{\ell} N(k,s-1,\boldsymbol{i})$$

Theorem [Dick-F. 2021]

- Startup cost of computing $M_{m,m'}(f,\mathcal{X})$ is $\mathcal{O}(sm'b^{m'}N)$
- Recomputing $M_{m,m'}(f,\mathcal{X})$ for the same data points $\mathcal{X}$ but different f costs $\mathcal{O}(sb^{m'})$

Error estimation

Walsh functions $w_k(x) := \exp(2\pi/b(k_0x_1 + \ldots + k_{j-1}x_j)$



Multidimensional analog

$$w_{\boldsymbol{k}}(x) := \prod_{j=1}^{s} w_{k_s}(x_s)$$

- $L^2([0,1]^s)$-orthogonal basis
- good to approximate smooth functions [Dick 2013]

Error estimation

Goal: approximate

$$\frac{1}{N}\sum_{n=1}^{N} c_n f(x_n) \approx \frac{1}{N}\sum_{n=1}^{N} c_n f_K(x_n) = \int_{[0,1]^s} f_K \phi_K \, dx = \int_{[0,1]^s} f \phi_K \, dx$$

- Walsh series approximation

$$f(x) \approx f_K(x) := \sum_{\boldsymbol{k}\in K} f_{\boldsymbol{k}} w_{\boldsymbol{k}}(x)$$

- approximate data density

$$\phi_K(x) := \sum_{\boldsymbol{k}\in K} \frac{1}{N}\sum_{n=1}^{N} c_n w_{\boldsymbol{k}}(x_n)\overline{w_{\boldsymbol{k}}}(x)$$

Error estimation

Goal: approximate

$$\frac{1}{N}\sum_{n=1}^{N} c_n f(x_n) \approx \frac{1}{N}\sum_{n=1}^{N} c_n f_K(x_n) = \int_{[0,1]^s} f_K \phi_K \, dx = \int_{[0,1]^s} f \phi_K \, dx$$

- use digital net to approximate integral

$$\int_{[0,1]^s} f \phi_K \, dx \approx b^{-m} \sum_{k=1}^{b^m} f(z_k)\phi_K(z_k)$$

- choose $K := \bigcup_{|\boldsymbol{d}|=m'} \{\boldsymbol{a} \,:\, \boldsymbol{a} \leq b^{\boldsymbol{d}}\}$ for

$$b^{-m} \sum_{k=1}^{b^m} f(z_k)\phi_K(z_k) = M_{m,m'}(f, \mathcal{X})$$

Error estimation

$$\frac{1}{N}\sum_{n=1}^{N} c_n f(x_n) \approx \int_{[0,1]^s} f\phi_K\,dx \approx b^{-m}\sum_{k=1}^{b^m} f(z_k)\phi_K(z_k)$$

Two approximation errors

- Walsh series approximation error

$$\|f - f_K\|_{L^\infty([0,1]^s)} \lesssim m'^q b^{-m'}\|f\|$$

- quadrature error for order α digital nets

$$\Big|\int_{[0,1]^s} f\phi_K\,dx - b^{-m}\sum_{k=1}^{b^m} f(z_k)\phi_K(z_k)\Big| \lesssim m^q b^{-\alpha(m-m')}\|f\|$$

Main result [Dick-F. 2021]

New algorithm to approximate large sums with QMC

$$\frac{1}{N}\sum_{n=1}^{N} c_n f(x_n) \approx M_{m,m'}(f,\mathcal{X})$$

- optimal choice $m' \simeq m/(1+1/\alpha)$ leads to

$$\left|\frac{1}{N}\sum_{n=1}^{N} c_n f(x_n) - M_{m,m'}(f,\mathcal{X})\right| \lesssim b^{-\alpha m/(1+\alpha)}$$

- with startup cost

$$\mathcal{O}(N b^{m/(1+\alpha)})$$

- and online cost

$$\mathcal{O}(b^m)$$

Remarks on main result

If data is QMC pointset $\implies \phi_K = 1 \implies \text{error} \lesssim b^{-\alpha m}$ [Longo, Mishra, Rusch, Schwab, 2021]

All error estimates depend on $\|f\|$

$$\partial_{\mathcal{W}_1,\dots,\mathcal{W}_k} f$$

- can be calculated explicitely for feed-forward networks
- use holomorphic activation function

$$\phi(x) = \tanh(x), \frac{x}{1+e^{-x}}, \frac{e^x}{1+e^x}$$

- can be controlled in terms of $\|\mathcal{W}\|$ [Longo, Mishra, Rusch, Schwab, 2021]

Finding good digital nets

most challenging part

$$\int_{[0,1]^s} f \phi_K \, dx$$

- f is smooth
- ϕ_K is piecewise constant Walsh expansion of order m'

$\implies$ (t, m, s)-net with $m - t \geq m'$ will integrate ϕ_K exactly

- if $m - t < m'$, approximation is bad
- strict limits on t-value of nets [Niederreiter-Xing]

$$t \gtrsim s - \log(s)$$

Weighted spaces?

Weighted spaces solve the problem for smooth functions

- definition of weighted spaces [Sloan-Woźniakowski 1998]

$$-\mathrm{div}(A(\boldsymbol{y})\nabla u) = f$$

Anisotropic expansion

$$A(x, \boldsymbol{y}) := \phi_0(x) + \sum_{i=1}^{\infty} y_i \phi_i(x)$$

leads to anisotropic derivatives

$$\|\partial_{y_{i_1} \ldots y_{i_k}} u\| \lesssim \Gamma_k \prod_{j=1}^{k} \gamma_{i_j}$$

$\implies$ t-value independent computation of $\mathbb{E}(G(u))$ in high-dimensions

Weighted (t, m, s)-nets?

- Digital nets with product and/or order dependent t-values

$$\Pi_{i_1,\ldots,i_k} P \quad \text{is } (t(i_1,\ldots,i_k), m, s)\text{-net}$$

- If ϕ_K of order m' represents data (images, . . .)

$$\int_{[0,1]^s} f\phi_K \, dx \approx \frac{1}{N} \sum_{i=1}^{b^m} f(z_i)\phi_K(z_i)$$

with $m \simeq m'$ "independent" of t-values

Weighted (t, m, s)-nets?

- digital nets are created via generator matrices

$$z_{m,j} = C_j \boldsymbol{m} \quad \text{in base } b$$

- t-value is direct consequence of rank properties of C_j

$\Longrightarrow$ direct search is infeasible (or is it? [L. Paulin's talk])

- many digital net constructions have explicit formulas for t-values
  - Sobol' sets: $t - \mathrm{val}(\Pi_{i_1,\ldots,i_k} P) = \sum_{j=1}^{k} \deg(p_{i_j})$
  - Similar formulas for Niederreiter-Xing sets

Not enough for what we want: given weighted t-values, construct pointset P

First order approximation property

Walsh series expansion with $K := \bigcup_{|\boldsymbol{d}|=m'} \{\boldsymbol{a} : \boldsymbol{a} \leq b^{\boldsymbol{d}}\}$ leads to

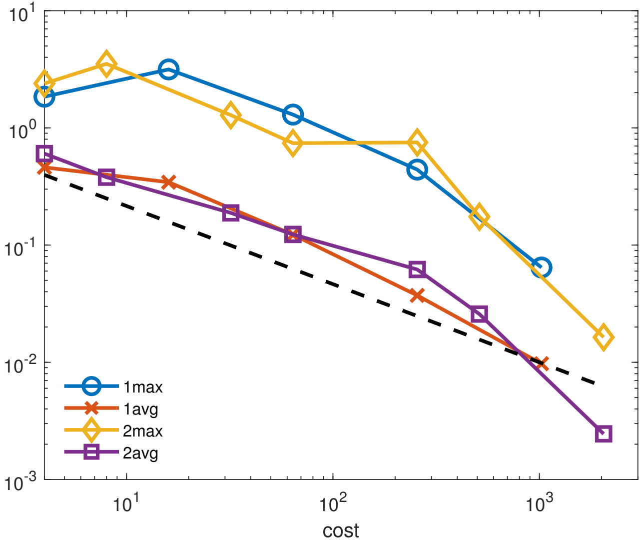
$$\|f - f_K\|_{L^\infty([0,1]^s)} \lesssim m'^q b^{-m'} \|f\|$$

- Can we improve that? $\mathcal{O}(b^{-\alpha m'})$
- Obviously: need larger $K \implies$ better digital nets which integrate ϕ_K exactly

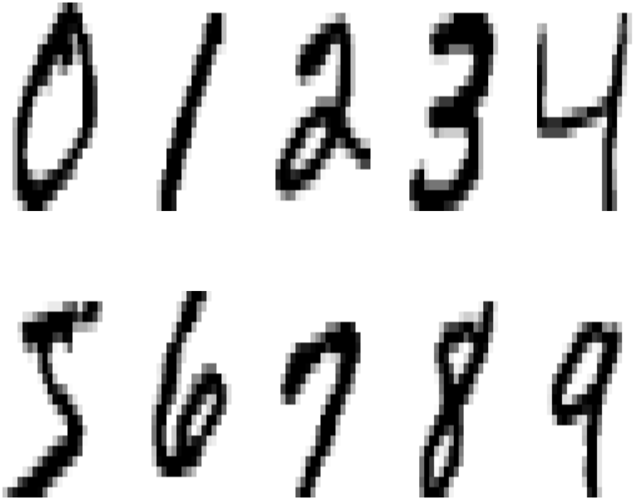
Similar results for "multiple rank-1 lattice rules"

- higher-order approximation with fourier series expansion
- [Kämmerer, Volkmer 2019], [Kämmerer 2016]

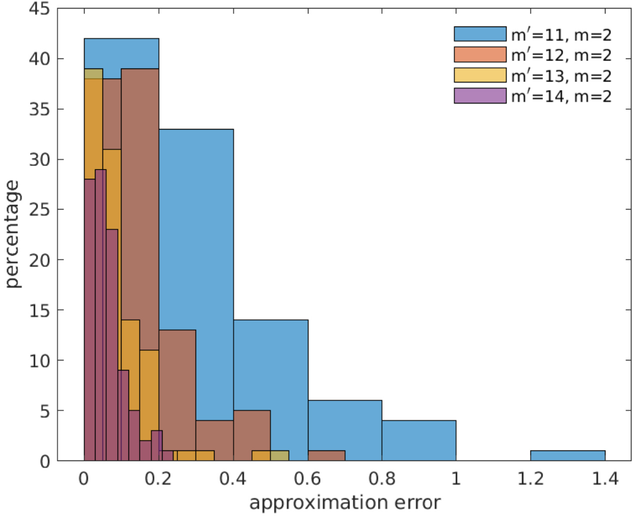
Numerical example: linear regression (6-dim)



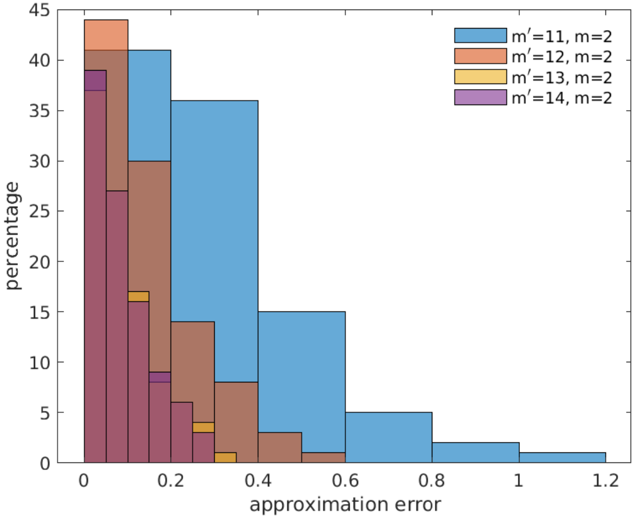
Numerical example: MNIST

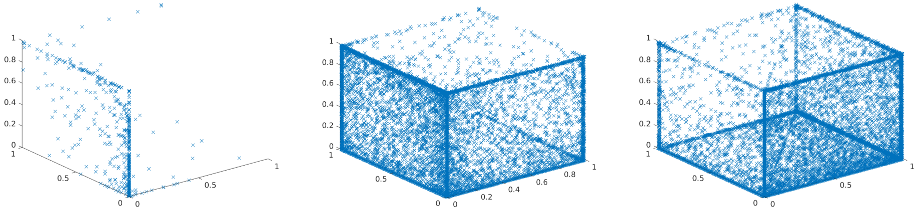


Numerical example: NN



Numerical example: DNN

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Thanks for Listening!

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