Optimizing Morse - Analytic Functions over Compact Domains

Journées Nationales de Calcul Formel 2024

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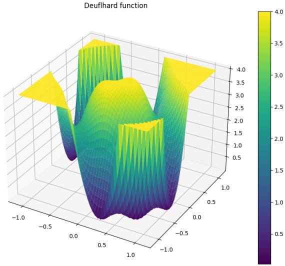

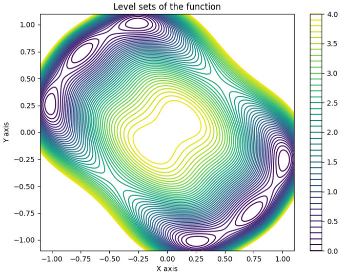

$$f(x,y) = \left(\exp(x^2+y^2) - 3\right)^2 + \left(x + y - \sin(3(x+y))\right)^2$$

Motivational Example

Global Optimization Problem

Given a smooth function f on a compact domain $\mathcal{C}_n \subset \mathbb{R}^n$, find *all* local minima of f located in the interior of $\mathcal{C}_n$.

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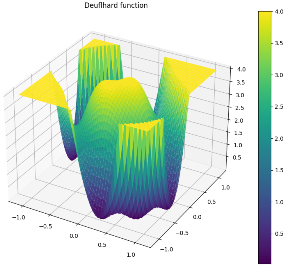

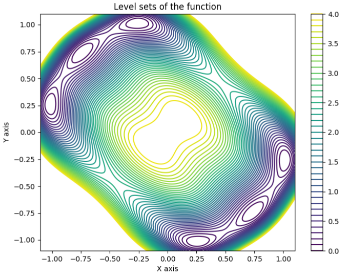

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Smooth Functions and Critical Points

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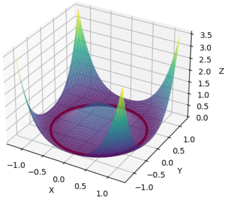

$$f = (x^2 + y^2 - 1)^2$$

Critical Points of Morse - Analytic Functions

Lemma

Let $f : \mathbb{R}^n \to \mathbb{R}$ be analytic on a neighborhood of x^*, an isolated local minimum of f in $\mathcal{C}_n$.
There exists an $r_0 > 0$ such that for any choice of $r \in (0, r_0]$, there is a constant $\epsilon > 0$ such that if a function g, analytic on the ball $B(x^*, r_0)$ satisfies

$$\|f - g\|_{L^2(B(x^*,r))} < \epsilon,$$

then g admits a local minimum in $B(x^*, r)$.

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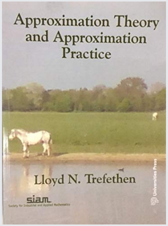

"Why are polynomial and rational approximations useful? Not because $r(x)$ is easier to evaluate than $\exp(x)$, but because [...] $r(\partial/\partial x)$ is easier to evaluate than $\exp(\partial/\partial x)$.
Not because we can evaluate $p(x)$, but because we can find its roots !"- N. Trefethen

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Let $\mathcal{P}_d \subset \mathbb{R}[x_1, \ldots, x_n]$ denote the space of real polynomials of degree at most d, of dimension $m = \binom{n+d}{d}$.
Accurately approximate f by a polynomial $u \in \mathcal{P}_d$.

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Initiate local minimization methods on f at each point in $\mathrm{crit}(u)$.

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$$e_d(f) = \|f - \mathcal{U}_d\|.$$

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Let G be the $m \times m$ Gramian matrix

$$G(\mathcal{S})_{j,k} = \langle L_j, L_k \rangle_{\mathcal{S}} = \frac{1}{K} \sum_{s \in \mathcal{S}} L_j(s) L_k(s). \tag{0.1}$$

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The solution to the normal equation

$$Gc = F \tag{0.2}$$

gives the coefficients of the polynomial $u_{d,\mathcal{S}} = \sum_{i=1}^{m} c_i L_i$.

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then we have

$$\mathbb{E}(\|f - u_{d,\mathcal{S}}\|^2) \leq (1 + \epsilon(K))\, e_d(f)^2 + 8\tau^2 K^{-r} \tag{0.4}$$

where $\epsilon(K) = \frac{4\kappa}{\ln K}$, which converges to 0 as K goes to infinity.

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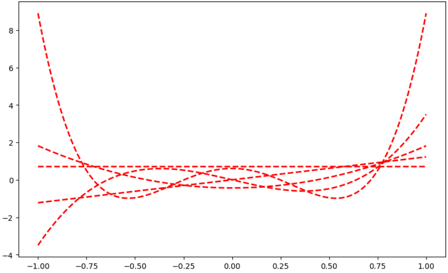

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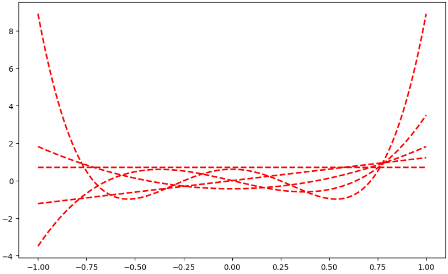

In that case, we have $sup_{x\in[-1,1]}|L_j(x)| = L_j(1) = \sqrt{1+2j}$. This requires a

$$k_m(x) = m^2 \leq \kappa \frac{K}{\ln(K)}$$

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Now we consider $L_1, \ldots, L_m$ an $L^2(\mathcal{C}_n, \rho)$ *orthonormal* basis of $\mathcal{P}_d$ and w a weight function such that $\int_{\mathcal{C}_n} w^{-1} d\rho = 1$.

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We sample $\mathcal{S}$ from μ and compute

$$u_{d,w,\mathcal{S}} = \underset{p \in \mathcal{P}_d}{\operatorname{argmin}} \left(\sum_{i=1}^{K} w(s_i) \left(p(s_i) - f(s_i) \right)^2 \right).$$

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$$(F_w)_j = \frac{1}{K} \sum_{i=1}^{K} w(s_i) f(s_i) L_j(s_i),$$

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The weighted version of the quantity previously defined,

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$$\sup_{x \in \mathcal{C}_n} k_{m,w}(x) \leq \kappa \frac{K}{\ln K}, \quad \kappa = \frac{1 - \ln 2}{2 + 2r},$$

then we have

$$\mathbb{E}(\|f - u_{d,w,\mathcal{S}}\|^2) \leq (1 + \epsilon(K))\, e_d(f)^2 + 8\tau^2 K^{-r}, \tag{0.7}$$

where $\epsilon(K) = \frac{4\kappa}{\ln K}$, which converges to 0 as K goes to infinity.

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We can restate the previous result as follows:

Corollary

For $r > 0$, if

$$m \leq \kappa \frac{K}{\ln K} \quad \text{where} \quad \kappa = \frac{1 - \ln 2}{2 + 2r},$$

then we have

$$\mathbb{E}(\|f - u_{d,\mathcal{S}}\|^2) \leq (1 + \epsilon(K))\, e_d(f)^2 + 8\tau^2 K^{-r}. \tag{0.8}$$

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3: $u_d \leftarrow \operatorname{argmin}_{p \in \mathcal{P}_d} \left(\frac{1}{K_d} \sum_{i=1}^{K_d} w(s_i)(p(s_i) - f(s_i))^2 \right)$

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6: $K_{check} \leftarrow \min \left\{ K \in \mathbb{N} \mid 2\binom{n+d}{d} \exp \left(-\frac{\zeta(\delta)K}{\binom{n+d}{d}} \right) \leq \mu \right\}$

7: $\tilde{\mathcal{S}} \leftarrow \{s_1, \dots, s_{K_{check}}\} \sim^{i.i.d.} \rho$

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For any given $r > 0$ and $d \in \mathbb{N}$

1: $K_d \leftarrow \min \left\{ K \in \mathbb{N} \mid \binom{n+d}{d} \leq \frac{1-\ln 2}{2+2r} \frac{K}{\ln K} \right\}$
2: $\mathcal{S}_1(d) \leftarrow \{s_1, \ldots, s_{K_d}\} \sim^{i.i.d.} \mu$
3: $u_d \leftarrow \operatorname{argmin}_{p \in \mathcal{P}_d} \left(\frac{1}{K_d} \sum_{i=1}^{K_d} w(s_i)(p(s_i) - f(s_i))^2 \right)$
4: $\mathcal{S}_2(d) \leftarrow \{s_1, \ldots, s_{2*K_d}\} \sim^{i.i.d.} \mu$, with $\mathcal{S}_1(d) \subseteq \mathcal{S}_2(d)$
5: $\tilde{u}_d \leftarrow \operatorname{argmin}_{p \in \mathcal{P}_d} \left(\|p - f\|_{\mathcal{S}_2(d)} \right)$
6: $K_{check} \leftarrow \min \left\{ K \in \mathbb{N} \mid 2\binom{n+d}{d} \exp\left(-\frac{\zeta(\delta)K}{\binom{n+d}{d}} \right) \leq \mu \right\}$
7: $\tilde{\mathcal{S}} \leftarrow \{s_1, \ldots, s_{K_{check}}\} \sim^{i.i.d.} \rho$
8: **if** $\|u_d - \tilde{u}_d\|_{\tilde{\mathcal{S}}} \geq \epsilon$ **then**

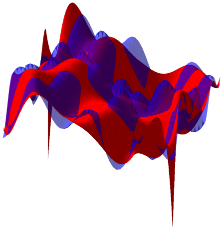
Our Method Summarized

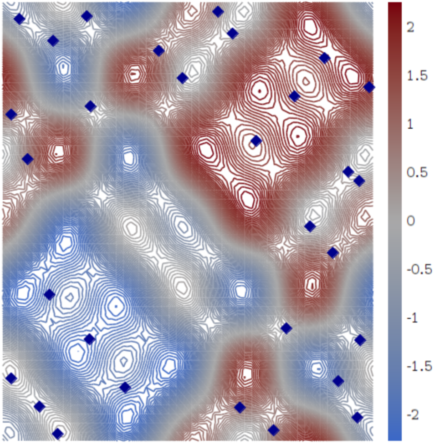
Set a relative error δ, a confidence level μ and a tolerance $\epsilon > 0$.
For any given $r > 0$ and $d \in \mathbb{N}$

1: $K_d \leftarrow \min \left\{ K \in \mathbb{N} \mid \binom{n+d}{d} \leq \frac{1-\ln 2}{2+2r} \frac{K}{\ln K} \right\}$
2: $\mathcal{S}_1(d) \leftarrow \{s_1, \ldots, s_{K_d}\} \sim^{i.i.d.} \mu$
3: $u_d \leftarrow \operatorname{argmin}_{p \in \mathcal{P}_d} \left(\frac{1}{K_d} \sum_{i=1}^{K_d} w(s_i)(p(s_i) - f(s_i))^2 \right)$
4: $\mathcal{S}_2(d) \leftarrow \{s_1, \ldots, s_{2*K_d}\} \sim^{i.i.d.} \mu$, with $\mathcal{S}_1(d) \subseteq \mathcal{S}_2(d)$
5: $\tilde{u}_d \leftarrow \operatorname{argmin}_{p \in \mathcal{P}_d} \left(\|p - f\|_{\mathcal{S}_2(d)} \right)$
6: $K_{check} \leftarrow \min \left\{ K \in \mathbb{N} \mid 2\binom{n+d}{d} \exp\left(-\frac{\zeta(\delta)K}{\binom{n+d}{d}} \right) \leq \mu \right\}$
7: $\tilde{\mathcal{S}} \leftarrow \{s_1, \ldots, s_{K_{check}}\} \sim^{i.i.d.} \rho$
8: **if** $\|u_d - \tilde{u}_d\|_{\tilde{\mathcal{S}}} \geq \epsilon$ **then**
9: $\quad K_d \leftarrow 2K_d$
10: $\quad \mathcal{S}_1(d) \leftarrow \mathcal{S}_2(d)$
11: $\quad u_d \leftarrow \tilde{u}_d$
12: $\quad$ Repeat from (4)
13: **end if**

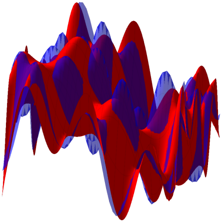
Example

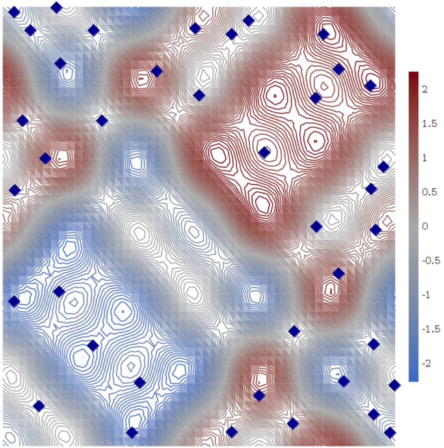
$$f(x) = \sin(10\pi x) + \sin(10\pi y) + \sin(20\pi x)\sin(20\pi y) - \cos(30\pi x)\cos(30\pi y)$$





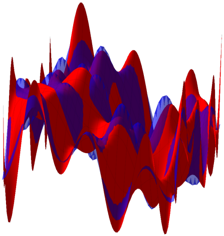
Example

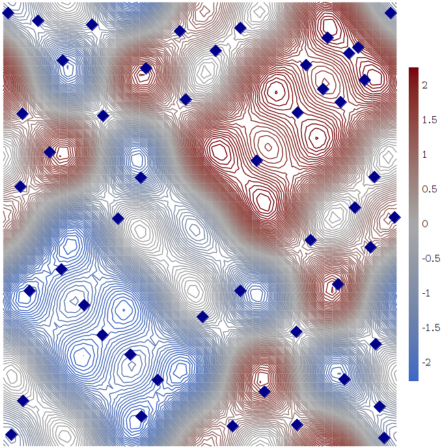




Least-squares approximant of degree 12 on $K = 10000$ samples.

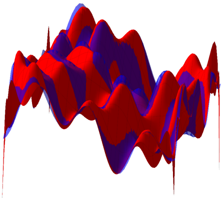
Example

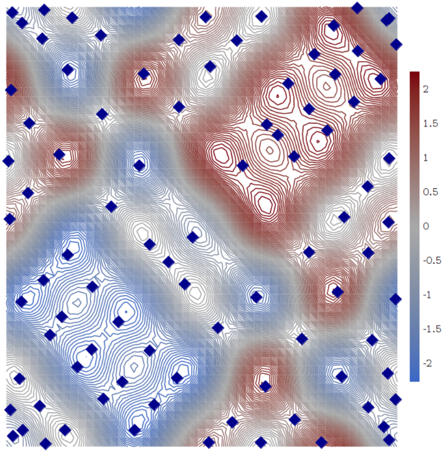




Least-squares approximant of degree 14 on $K = 10000$ samples.

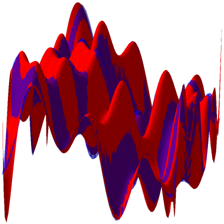
Example

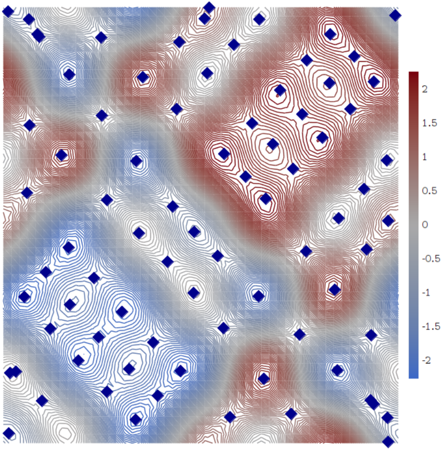




Least-squares approximant of degree 16 on $K = 10000$ samples.

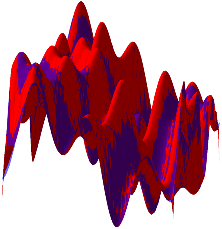
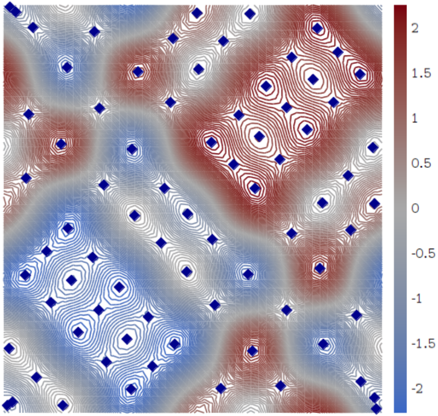
Example





Least-squares approximant of degree 18 on $K = 10000$ samples.

Example

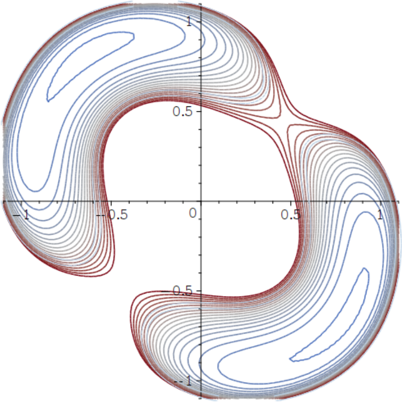



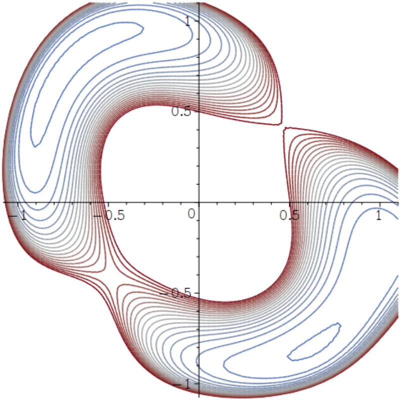
Least-squares approximant of degree 20 on $K = 10000$ samples.

Back To Deuflhard's Example

Back To Deuflhard's Example

Approximant constructed on $K = 200$ sample points.





Degree 8 approximant in Chebyshev basis, condition number of G_w: 57

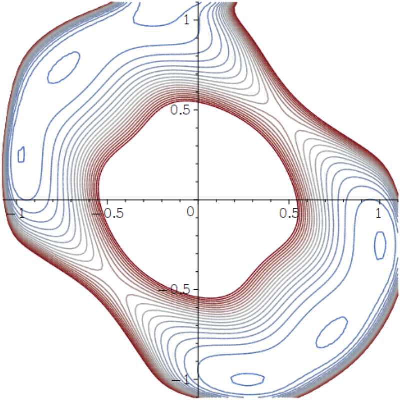
Degree 8 approximant in standard basis, condition number of G: $1.67 \cdot 10^5$

.

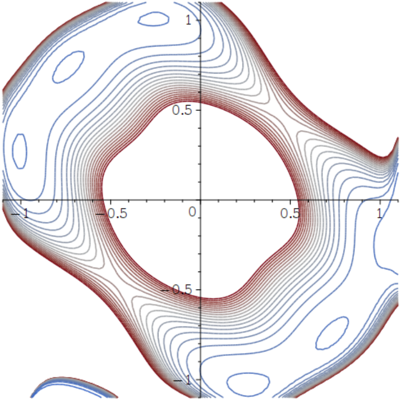
Back To Deuflhard's Example

Back To Deuflhard's Example

Approximant constructed on $K = 200$ sample points.



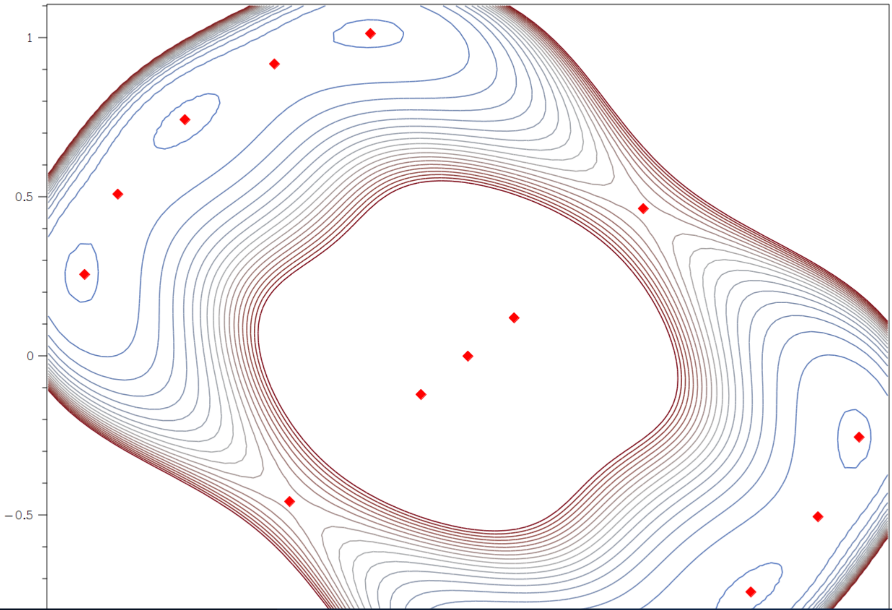
Degree 16 approximant in Chebyshev basis, condition number of G_w: $3.31 \cdot 10^6$



Degree 16 approximant in standard basis, condition number of G: $6.30 \cdot 10^{11}$

.

Back To Deuflhard's Example



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Discussions

Numerical stability of constructing Least-Squares approximants.

Maple LS Solve for larger examples.

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Numerical stability of constructing Least-Squares approximants.

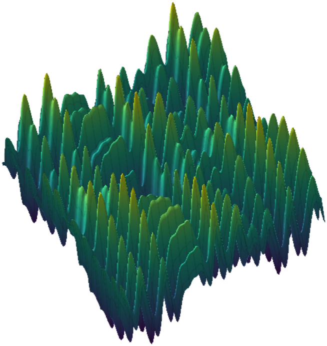
Lemma (Morse's Lemma)

Let $f \in \mathrm{crit}^\infty$ and $x^* \in \mathcal{C}_n$ be a non-degenerate critical point of f with $H_f(x^*)$ of index j. Then there exists $(x_1, \ldots, x_n)$ such that, on some small open neighborhood of x^*, we have

$$f(x) = f(x^*) - \sum_{i=1}^{j} x_i^2 + \sum_{i=j+1}^{n} x_i^2.$$

Maple LS Solve for larger examples.

A More Ambitious Example



$$f(x,y) = \exp^{\sin(50x)} + \sin(60\exp^{y})\sin(70\sin(x)) + \sin(\sin(80y)) - \sin(10(x+y)) + (x^2+y^2)/4. \quad (0.9)$$