Solvable Integration Problems and Optimal Sample Size Selection

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(joint work with Erich Novak and Daniel Rudolf)

UNIVERSITÄT OSNABRÜCK

Special Session: When to stop a simulation

MCQMC2018, mercredi, le 4 julliet 2018, Rennes

Standard Monte Carlo integration

Task: Compute $\mathbb{E}\, Y$ from random samples $Y_1, Y_2, \ldots \overset{\text{iid}}{\sim} Y$.

Standard Monte Carlo method:

$$\widehat{M}_n(Y) := \frac{1}{n} \sum_{i=1}^{n} Y_i$$

Application to integration w.r.t. prob. measure π on domain G, using $X, X_1, X_2, \ldots \overset{\text{iid}}{\sim} \pi$:

$$\mathrm{INT}\, f := \int_G f \,\mathrm{d}\pi \;\approx\; \widehat{M}_n(f(X)) \;=\; \frac{1}{n} \sum_{i=1}^{n} f(X_i)$$

Standard Monte Carlo error / root mean square error (RMSE):

$$e(\widehat{M}_n, Y) := \sqrt{\mathbb{E}\left(\widehat{M}_n(Y) - \mathbb{E}\, Y\right)^2} = \frac{\sigma(Y)}{\sqrt{n}}$$

Problem: What if variance $\sigma^2(Y)$ unknown?

Integration for a-priori unknown variance

Theorem (Hickernell, Jiang, Liu, Owen 2013)

Given $K > 1$, then for any error threshold $\varepsilon > 0$ and any uncertainty level $\delta > 0$, there exists an algorithm $A^K_{\varepsilon,\delta}$ such that

$$\mathbb{P}\left\{ |A^K_{\varepsilon,\delta}(Y) - \mathbb{E}\, Y| > \varepsilon \right\} \leq \delta$$

for all Y with bounded kurtosis, $\|Y - \mathbb{E}\, Y\|_4 \leq K \|Y - \mathbb{E}\, Y\|_2$.

Idea:

1. use fixed sample $Y_1, \ldots, Y_{n_1}$ for a variance estimate
2. choose size n_2 of sample $Y_{n_1+1}, \ldots, Y_{n_1+n_2}$ for mean estimate

There is no solution with fixed sample size!

Question: Optimality? Other assumptions? Mean squared error?

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Definition of solvability

Inputset $\mathcal{F} \subset L_1(\pi)$ — class of integrands f
with respect to prob. measure π on domain G

General randomized algorithm = mapping $A : \Omega \times \mathcal{F} \to \mathbb{R}$,
requiring only finitely many function evaluations, $n(\omega, f) < \infty$.

Special type: **i.i.d.-based algorithms** using $f(X_i)$ where $X_i \stackrel{\text{iid}}{\sim} \pi$

Definition (Solvable integration problems)

The integration problem is solvable for $\mathcal{F}$
iff for all $\varepsilon, \delta > 0$ exists an (ε, δ)-approximating algorithm A, i.e.

$$\mathbb{P}\{|A(f) - \mathrm{INT}\, f| > \varepsilon\} \leq \delta \qquad \text{for all } f \in \mathcal{F}.$$

Example of an unsolvable problem

Theorem (K., Novak, Rudolf 2018)

The integration problem $\int_0^1 f \, \mathrm{d}x$
is unsolvable for the class $\mathcal{F} = C^\infty([0,1])$.

Idea of the proof: How would you distinguish $f = 0$ from functions f with huge integral but small support? Impossible!

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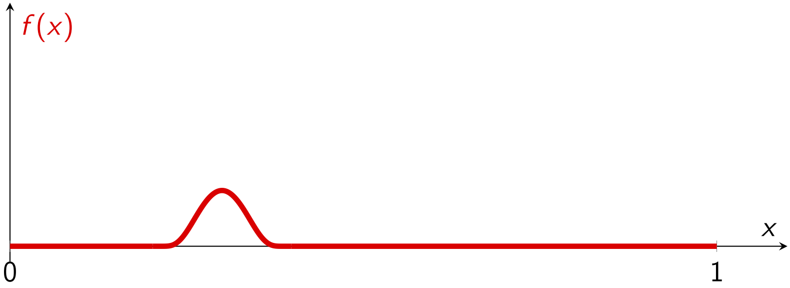

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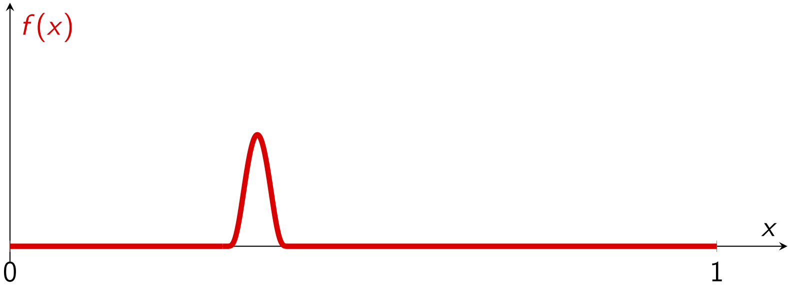

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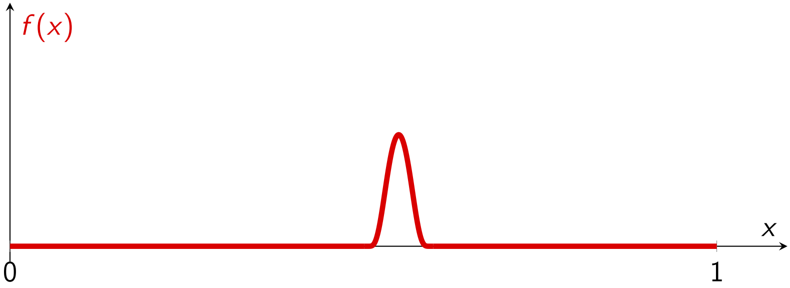

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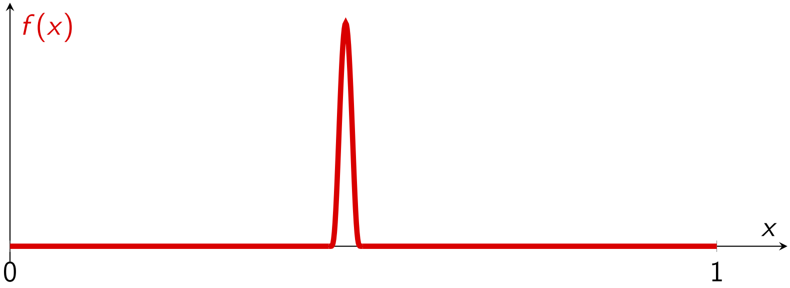

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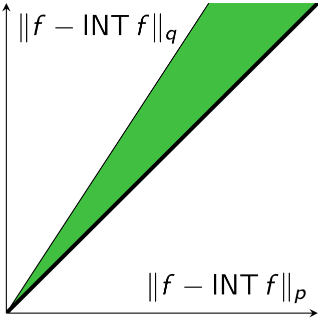
Generalizing the kurtosis – a cone-shaped input set

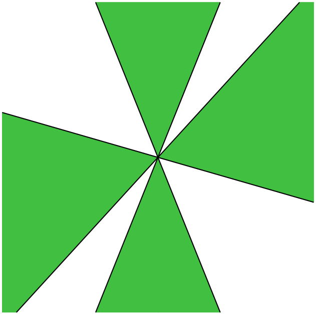
For $1 \leq p < q \leq \infty$ and $K > 1$, (Hickernell et al.: $p = 2$, $q = 4$)

$$\mathcal{F}_{p,q,K} := \{f \in L_q(\pi) \colon \|f - \mathrm{INT}\, f\|_q \leq K \|f - \mathrm{INT}\, f\|_p\}$$

Scaling property: $f \in \mathcal{F}_{p,q,K} \quad \Rightarrow \quad cf \in \mathcal{F}_{p,q,K}$ for all $c \in \mathbb{R}$.



cone condition



within 2-dim. subspace of L_q

Upper bound for the expected cost

Recall input set for $1 \leq p < q \leq \infty$ and $K > 1$,

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Theorem (K, Novak, Rudolf 2018)

For any error threshold $\varepsilon > 0$ and uncertainty level $\delta > 0$, there exists an (ε, δ)-approximating algorithm $A_{\varepsilon,\delta}^{p,q,K}$ on $\mathcal{F}_{p,q,K}$. Writing $\widetilde{q} := \min\{q, 2\}$, the expected sample size $\bar{n}$ is bounded by

$$\bar{n}(A_{\varepsilon,\delta}^{p,q,K}, f) := \mathbb{E}\, n(\omega, f)$$

$$\leq \left[C_q\, K^{pq/(q-p)} + C_{q,K} \left(\frac{\|f - \mathrm{INT}\, f\|_1}{\varepsilon} \right)^{1+1/(\widetilde{q}-1)} \right] \log \frac{1}{\delta} .$$

Structure of the algorithm

Parameters: odd $k, k' \in \mathbb{N}$; $2 \leq m \in \mathbb{N}$; $1 < \eta \in \mathbb{R}$.

Information: random samples $Y_i := f(X_i)$ with $X_1, X_2, \ldots \overset{\text{iid}}{\sim} \pi$

1. estimate $\|f - \mathrm{INT}\, f\|_1$ from $n_1 := k \cdot m$ observations:

$$\widehat{R}_{k,m} := \mathrm{med}(\widehat{R}_m^{(1)}, \ldots, \widehat{R}_m^{(k)}), \quad \text{where}$$

$$\widehat{R}_m^{(\ell)} \overset{\text{iid}}{\sim} \frac{1}{m} \sum_{i=1}^{m} |Y_i - \widehat{M}_m|, \quad \text{with} \quad \widehat{M}_m := \frac{1}{m} \sum_{i=1}^{m} Y_i$$

2. estimate $\mathrm{INT}\, f$ via $n_2 := k' \cdot m'$ additional observations, $m' := \max\{\lceil \eta\, (\widehat{R}_{k,m})^{1+1/(\tilde{q}-1)} \rceil, 1\}$, with $\tilde{q} := \min\{q, 2\}$,

$$A_{k,m}^{k',\eta,\tilde{q}}(f) := \mathrm{med}(\widetilde{M}_{m'}^{(1)}, \ldots, \widetilde{M}_{m'}^{(k')}), \quad \text{where} \quad \widetilde{M}_{m'}^{(\ell)} \overset{\text{iid}}{\sim} \widehat{M}_{m'}$$

Median trick $\rightsquigarrow$ probability amplification, finite expected cost

Alternative for 1 on $\mathcal{F}_{p,q,K}$: if $q \leq 2$, estimate $\|f - \mathrm{INT}\, f\|_p^p$,
if $2 < q$, estimate $\|f - \mathrm{INT}\, f\|_2^2$.

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An absolute lower bound – the fixed cost

Theorem (K, Novak, Rudolf 2018)

Any (ε,δ)-approximating algorithm $A_{\varepsilon,\delta}$ on $\mathcal{F}_{p,q,K}$ requires a minimal amount of information, irrespective of the input,

$$\bar{n}^{\mathrm{fix}}(\varepsilon,\delta,\mathcal{F}_{p,q,K}) := \inf_{A_{\varepsilon,\delta}} \inf_{f\in\mathcal{F}_{p,q,K}} \bar{n}(A_{\varepsilon,\delta},f) \geq \frac{1}{2\log 2}\, K^{pq/(q-p)} \log\frac{1}{2\delta}\,.$$

Proof: Distinguish $f \in \mathcal{F}_{p,q,K}$ from perturbed $f+h \in \mathcal{F}_{p,q,K}$, where $h \in \mathcal{F}_{p,q,K}$ with $\pi\{h=c\} = 1-\pi\{h=0\} \in (0,\frac{1}{2})$?

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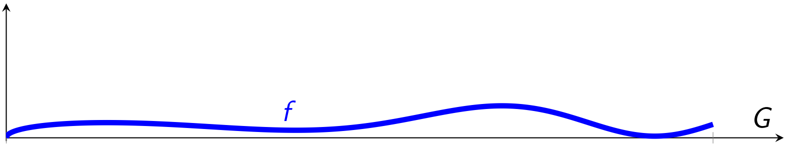

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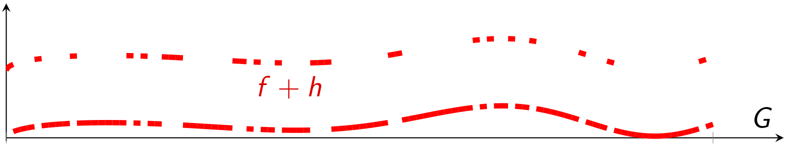

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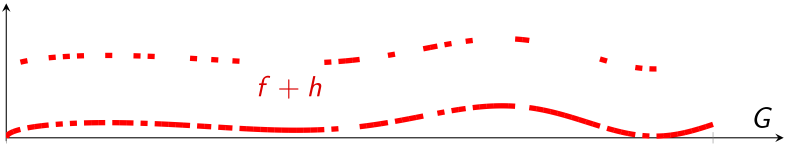

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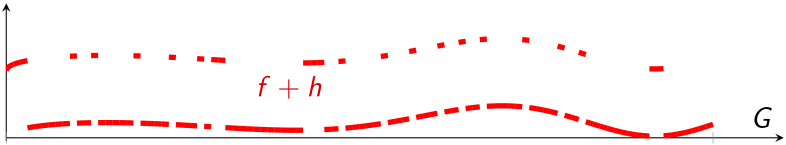

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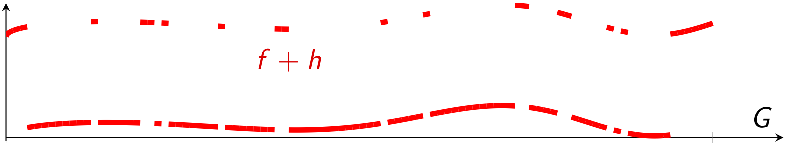

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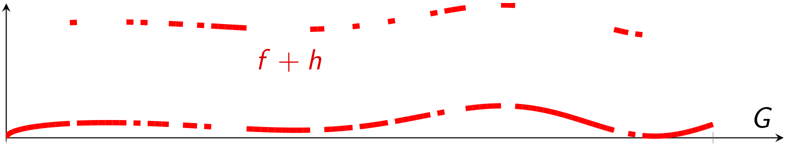

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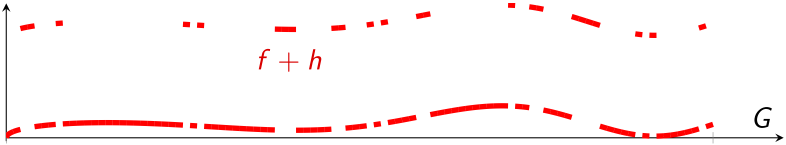
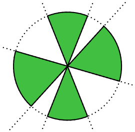


Worst case cost for bounded norm

Put $\widetilde{q} := \min\{q, 2\}$, we intersect $\mathcal{F}_{p,q,K}$ with

$$\tau\mathcal{B}_{\widetilde{q}} := \{f \in L_{\widetilde{q}}(\pi) : \|f - \mathrm{INT}\, f\|_{\widetilde{q}} \leq \tau\}$$



Theorem (K, Novak, Rudolf 2018)

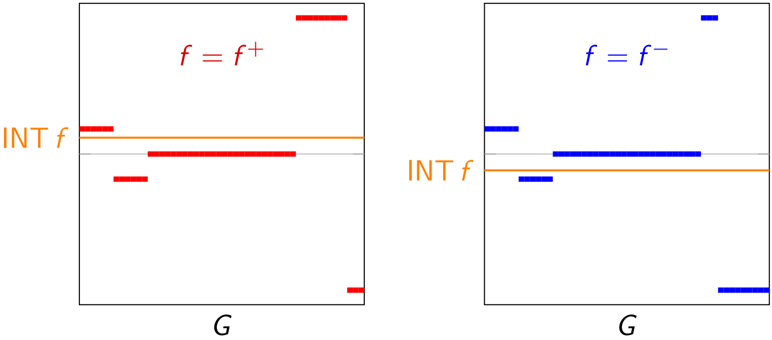
For any (ε, δ)-approximating algorithm $A_{\varepsilon,\delta}$ on $\mathcal{F}_{p,q,K}$, the worst case cost for $\|f - \mathrm{INT}\, f\|_{\widetilde{q}} \leq \tau$ is bounded below by

$$\bar{n}^{\mathrm{wor}}(\varepsilon, \delta, \mathcal{F}_{p,q,K} \cap \tau\mathcal{B}_{\widetilde{q}}) := \inf_{A_{\varepsilon,\delta}} \sup_{f \in \mathcal{F}_{p,q,K} \cap \tau\mathcal{B}_{\widetilde{q}}} \bar{n}(A_{\varepsilon,\delta}, f)$$
$$\geq c_{q,K} \left(\frac{\tau}{\varepsilon}\right)^{1+1/(\widetilde{q}-1)} \log \frac{3}{4\delta}$$

for error thresholds $0 < \varepsilon < C_K \tau$ and uncertainty $0 < \delta \leq \frac{1}{4}$.

Worst case cost for bounded norm – proof

Worst case lower bounds on $\mathcal{F}_{p,q,K} \cap \tau\mathcal{B}_{\tilde{q}}$ using i.i.d. $Y_i := f(X_i)$
via cost bounds for statistical tests (Wald 1945) $\rightsquigarrow$ f^+ vs. f^-?



Same lower bounds for general algorithms using function values,
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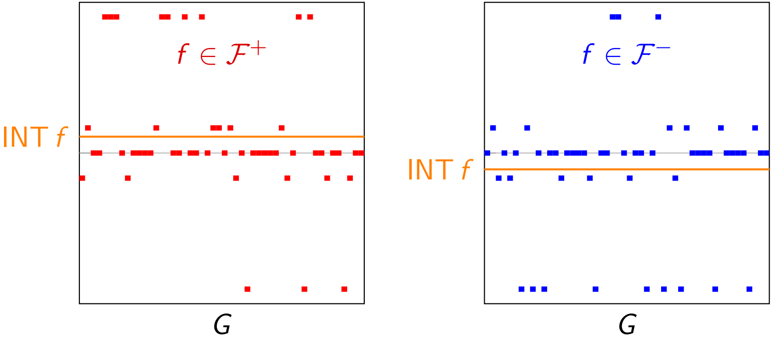

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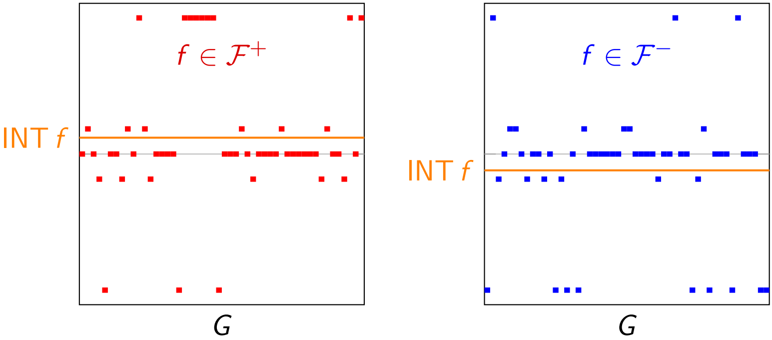

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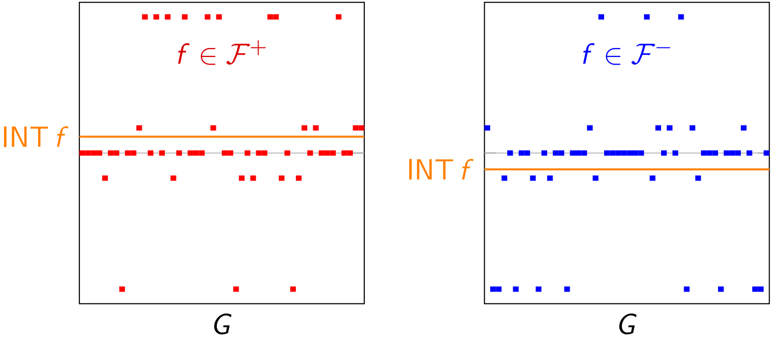

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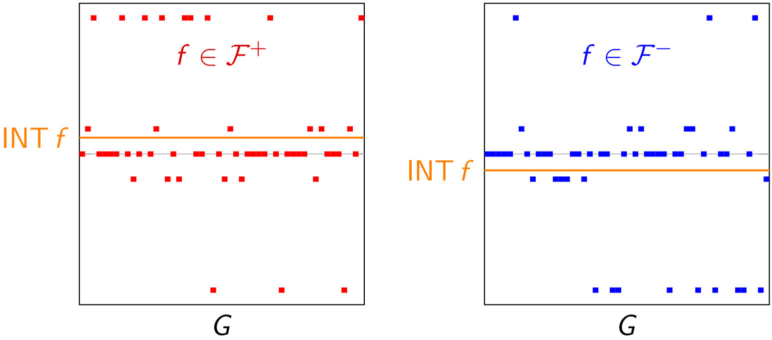
Worst case cost for bounded norm – proof

Worst case lower bounds on $\mathcal{F}_{p,q,K} \cap \tau\mathcal{B}_{\widetilde{q}}$ using i.i.d. $Y_i := f(X_i)$ via cost bounds for statistical tests (Wald 1945) $\rightsquigarrow$ f^+ vs. f^-?



Same lower bounds for general algorithms using function values, if π has no atoms $\rightsquigarrow$ distinguish shuffled classes $\mathcal{F}^+$ and $\mathcal{F}^-$

Summary

Input set for $1 \le p < q \le \infty$ and $K > 1$, $\tilde{q} := \min\{q, 2\}$

$$\mathcal{F}_{p,q,K} := \{f \in L_q(\pi) \colon \|f - \mathrm{INT}\, f\|_q \le K \|f - \mathrm{INT}\, f\|_p\}$$

Upper bound for (ε, δ)-approximating algorithm $A_{\varepsilon,\delta}^{p,q,K}$ on $\mathcal{F}_{p,q,K}$

$$\bar{n}(A_{\varepsilon,\delta}^{p,q,K}, f) \le C_{q,K} \left[1 + \left(\frac{\|f - \mathrm{INT}\, f\|_1}{\varepsilon}\right)^{1+1/(\tilde{q}-1)}\right] \log \frac{1}{\delta}$$

Fixed cost – an absolute lower bound

$$\bar{n}^{\mathrm{fix}}(\varepsilon, \delta, \mathcal{F}_{p,q,K}) \ge \frac{1}{2 \log 2} K^{pq/(q-p)} \log \frac{1}{2\delta}$$

Worst case cost for $\|f - \mathrm{INT}\, f\|_{\tilde{q}} \le \tau$,

$$\bar{n}^{\mathrm{wor}}(\varepsilon, \delta, \mathcal{F}_{p,q,K} \cap \tau \mathcal{B}_{\tilde{q}}) \ge c_{q,K} \left(\frac{\tau}{\varepsilon}\right)^{1+1/(\tilde{q}-1)} \log \frac{3}{4\delta}$$

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