The Multilevel Monte Carlo Method: basic concepts and further developments

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The Monte Carlo Method

Question: Suppose X is a Random Variable, such that

- X is not available in closed form
- X is available through its i.i.d. samples X^i

How to compute accurately and and quickly the mean value

$$\mu = \mathbb{E}[X] = \int_\Omega X(\omega)\,\mathrm{d}\mathbb{P}(\omega) \qquad ?$$

Monte Carlo: Use sample average:

$$E_M[X] := \frac{1}{M}\sum_{i=1}^{M} X^i.$$

How good is this approximation? $Z := E_M[X] - \mu = ?$

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$$\mathrm{MSE} = \mathbb{E}\left[Z^2\right], \qquad Z = E_M[X] - \mu.$$

Theorem

$$\mathrm{MSE} = \frac{1}{M}\,\mathrm{Var}[X].$$

Drawbacks:

- Very slow (Root-$\mathrm{MSE} \sim \frac{1}{\sqrt{M}}$)
- Usually not realistic: approximate samples of $X_N \approx X$.

Here N is a „discretization parameter“, e.g.

- # particles in a MD-Simulation
- # dof in a Finite Element / Finite Difference approximation
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- Still very slow and expensive (halving the bias $\leftrightarrow$ quadrupling M)
- In particular, if
  - Approx. error $\sim N^{-\alpha}$
  - $\mathrm{Cost}(X_N) \sim N^{\gamma}$

  Then $\mathrm{RMSE} \sim \varepsilon$ for the $\mathrm{Cost} \sim \varepsilon^{-2-\frac{\gamma}{\alpha}}$.

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$$E^{ML}[X] := E_M[X_N - X_n] + E_M[X_n], \qquad n < N.$$

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($m < M$: faster sampling for the same accuracy)

Extension to multiple levels $\Rightarrow$ **Multilevel Monte Carlo**

$$E^{ML}[X] := \sum_{\ell=1}^{L} E_{M_\ell}[X_\ell - X_{\ell-1}], \qquad X_0 = 0.$$

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Main idea: Equidistrib. of the comput. cost over FE levels

1. Heinrich, J. Complexity (1998)
2. Giles, Oper. Res. (2008)
3. Barth, Schwab, Zollinger, Numer. Math. (2011)
4. Cliffe, Giles, Scheichl, Teckentrup, Comput. Vis. Sci. (2011)

...

Our work [Bierig/Chernov'15+]:

- Multilevel MC approx. of the variance and higher order moments

$$\mu^k = \mathbb{E}(X - \mathbb{E}[X])^k = \int_{-\infty}^{\infty} (x-\mu)^k f_X(x)\, dx,$$

- Approximation of Probability Density Functions f_X via Max. Entropy Method

$$f_X \approx \operatorname{argmin} \left\{ \int \rho \ln \rho \ : \ \mu^k = \int (x-\mu)^k \rho(x)\, dx \right\}$$

- Application to the contact with rough random obstacles.

Multilevel Monte Carlo sample mean estimator:

$$\mathbb{E}[X] \approx E^{ML}[X] = \sum_{\ell=1}^{L} E_{M_\ell}[X_\ell - X_{\ell-1}], \qquad X_0 = 0.$$

Theorem (Accuracy / Cost relation, simplified)

Assume that

a) $|\mathbb{E}[X - X_\ell]| \lesssim N_\ell^{-\alpha}$, b) $\mathrm{Var}[X_\ell - X_{\ell-1}] \lesssim N_\ell^{-\beta}$, c) $\mathrm{Cost}(X_\ell) \lesssim N_\ell^{\gamma}$,

then there exist M_ℓ, s.t. $\mathrm{RMSE}(E_M) < \varepsilon$ and $\mathrm{RMSE}(E^{ML}) < \varepsilon$

$$\mathrm{Cost}(E_M) \lesssim \varepsilon^{-2-\frac{\gamma}{\alpha}}, \qquad \mathrm{Cost}(E^{ML}) \lesssim \varepsilon^{-2-\frac{\gamma}{\alpha}+\frac{\min(2\alpha,\beta,\gamma)}{\alpha}}. \qquad (\gamma \neq \beta)$$

Proof (sketch for the case $2\alpha > \min(\beta,\gamma)$):

- $\mathrm{MSE}(E^{ML}) = |\mathbb{E}[X_L - X]|^2 + \sum_{\ell=1}^{L} \frac{1}{M_\ell} Var[X_\ell - X_{\ell-1}] \sim \varepsilon^2$

- Balancing the summands: $N_L^{-2\alpha} \sim \varepsilon^2$ and $\sum_{\ell=1}^{L} \frac{N_\ell^\beta}{M_\ell} \sim \varepsilon^2$

- Finding M_ℓ : Minimize $\mathrm{Cost}(E^{ML})$ under constraints ↑

$$\mathrm{Cost}(E^{ML}) \sim \sum_{\ell=1}^{L} M_\ell \cdot \mathrm{Cost}(X_\ell)$$

- Optimal choice: $M_\ell \sim N_\ell^{-\frac{\beta+\gamma}{2}} \Rightarrow \mathrm{Cost}(E^{ML}) \sim \sum_{\ell=1}^{L} N_\ell^{\frac{\gamma-\beta}{2}}$

$\rightarrow\ \beta > \gamma \Rightarrow \ell = 1$ is dominating $\Rightarrow \mathrm{Cost}(E^{ML}) \sim M_0 N_0^\gamma \sim \varepsilon^{-2}$,

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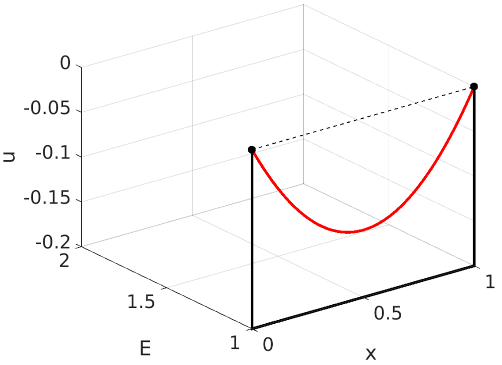
Homework: complete this proof. □

Examples

Model: Wire rope (e.g. overhead power line) in equilibrium

$$-u''(x) = f, \quad \text{for} \quad 0 < x < 1 \qquad f = \text{gravitation force (const.)}$$
$$u(0) = 0, \qquad u = \text{vertical displacement}$$
$$u(1) = 0.$$



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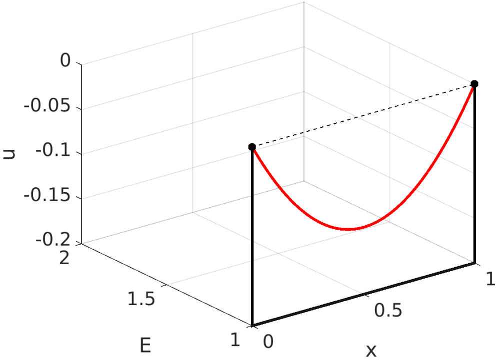

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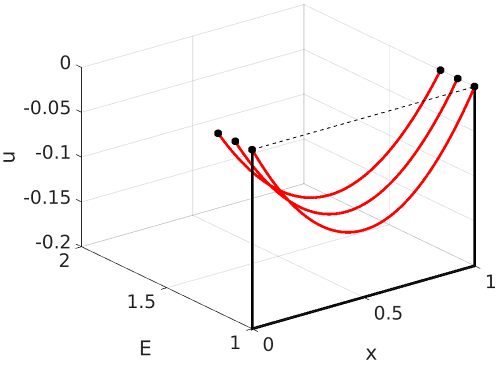

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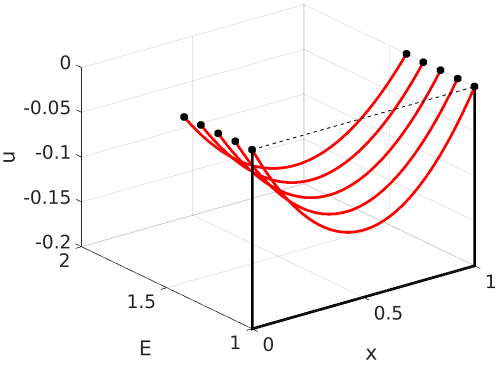

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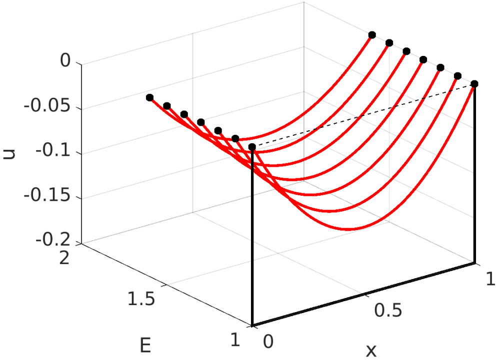

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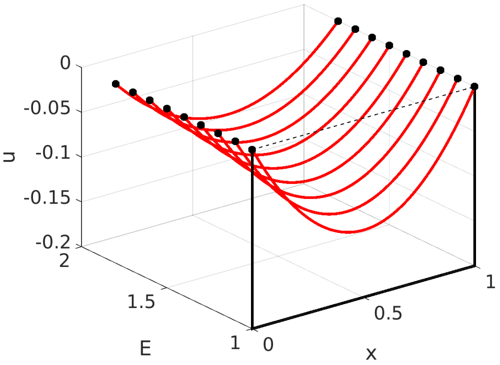

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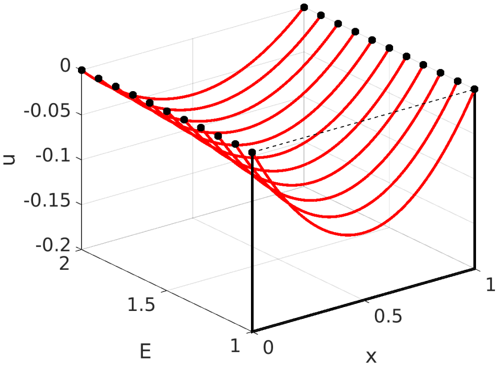

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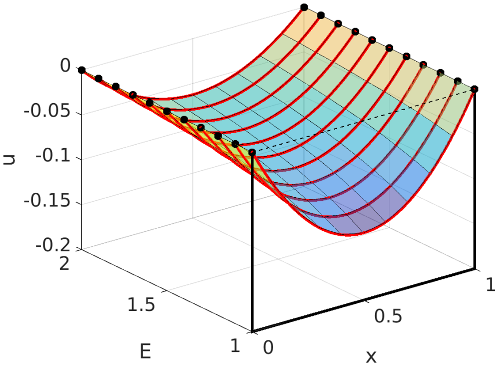

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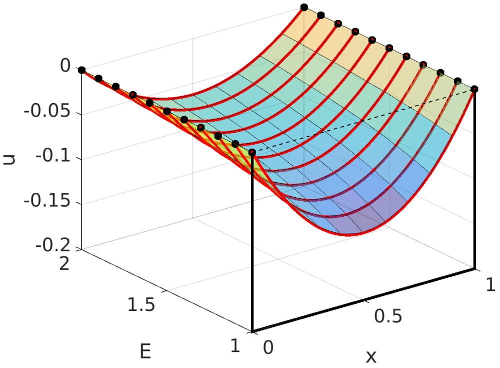

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When E is variable, u can be viewed as a function of x and E.

The variation of E describes e.g. different materials.

Example: Wire rope (conductor) in the electrical overhead line:

- Aluminium
- Steel
- Copper
- Alloys (Aldrey: 99% Al + 0.5% Mg + 0.5% Si)

Variations of the proportion $\Rightarrow$ Variations of E.

Typical problem in forward uncertainty propagation

Assuming that statistical variations of E can be estimated in the fabrication process, is it possible to find probabilistic properties of the wire rope?

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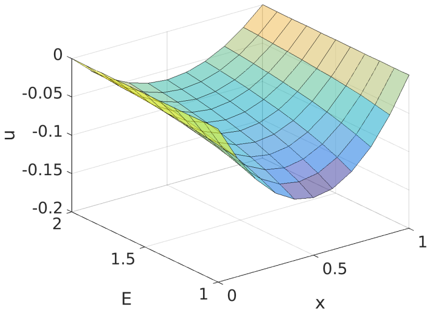

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check these relations!

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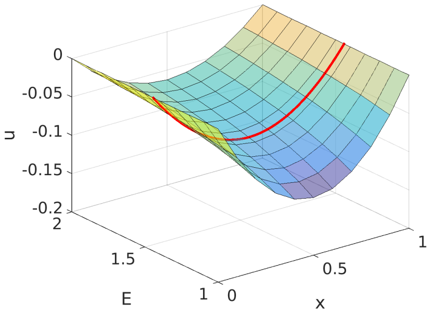

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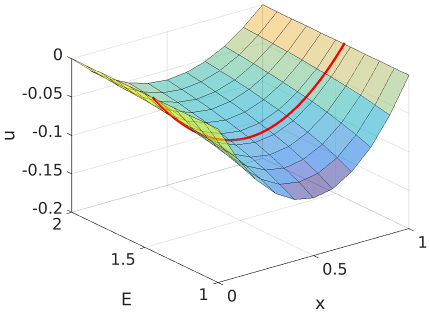

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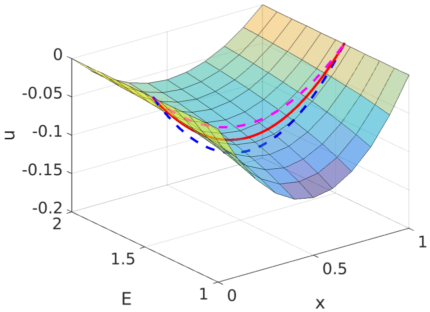

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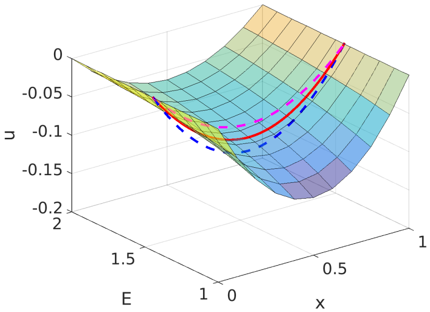

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Correl. Coefficient: $$r(x,y) = \frac{\mathrm{Cov}[u](x,y)}{\sigma(x)\sigma(y)} = 1, \quad \text{(perfect Correlation)}$$

Probability Density Function: $$\rho_{u(x)}(t) \propto \frac{1}{t^2}, \qquad \frac{1}{2} \leq t \leq 1.$$

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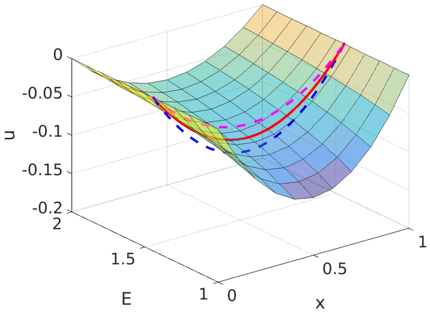

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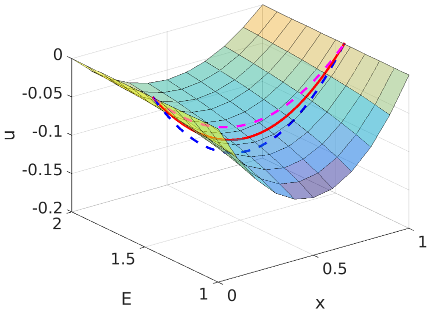

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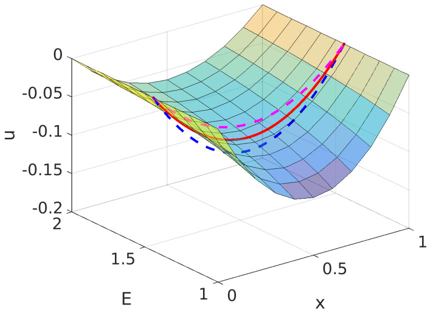

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This is very rare in praxis! The model problem was just too simple:

- The physical domain $D = (0, 1)$ was one-dimensional;
- E was homogeneous. What if $E = E(x, \omega)$ varies in space?
- The material law was very simple;
- The solution operator was smooth ...

In practical applications exact evaluation of $u(x, E)$ is out of reach.

Computer approximations:

$$u(x, E) \approx u_N(x, E) = S_N(E)$$

Is it still possible to **approximately** compute **probabilistic properties** of the exact solution $u(x, E)$?

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Examples of uncertain parameters in applications

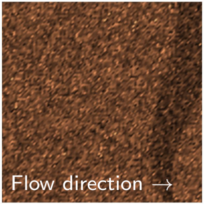
1) Pollution in groundwater flow model:

$$\begin{cases} \mathbf{q} = -K\nabla p & \text{Darcy's law} \\ \nabla \cdot \mathbf{u} = 0 & \text{Mass conservation} \\ \mathbf{q} = \phi \mathbf{u} & \end{cases}$$

$\mathbf{q}$: Darcy flux, K : conductivity, p : pressure
$\mathbf{u}$: pore velocity, ϕ : porosity, $\mathbf{x}$: position

Particle transport

$$\begin{cases} \dfrac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}) \\ \mathbf{x}(\mathbf{0}) = \mathbf{x}_0 \end{cases}$$



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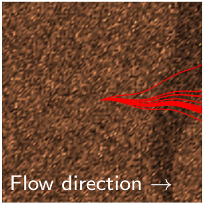

Random conductivity
$K = K(\mathbf{x}, \omega)$

Qty of interest:
$T(\omega) = \max\{t : \mathbf{x}(\omega) \in \mathbf{D}\}$
(particle travel time),
$\mathbb{E}[T]$, $\mathbb{V}[T]$

Examples of uncertain parameters in applications

2) Elastic deformation of random media

$$\begin{cases} \mathrm{div}\sigma + \vec{f} = 0 & \text{Equilibrium eq.} \\ \sigma_{ij} = \dfrac{E}{1+\nu}\left(\dfrac{\nu\delta_{ij}\varepsilon_{kk}}{1-2\nu} + \varepsilon_{ij}\right) & \text{Constitutive eq.} \\ \varepsilon = \dfrac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^\top) & \end{cases}$$

σ : stress, ε : strain, $\mathbf{u}$: displacement,
$\vec{f}$: volume forces, E : Young's Modulus, ν : Poisson's ratio

Random material parameters:

$$E = E(\mathbf{x}, \omega), \quad \nu = \nu(\mathbf{x}, \omega),$$

Qty of interest:

$$\sigma_{\max}(\omega) = \max_{\mathbf{x} \in D}\{\|\mathrm{dev}\sigma\|_F\}$$

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---

3) + elasto-plastic deformations: $f_{pl} = \|\mathrm{dev}\sigma\|_F - \sqrt{\frac{2}{3}}\sigma_Y \leq 0$

Random yield stress: $\sigma_Y = \sigma_Y(\mathbf{x}, \omega)$

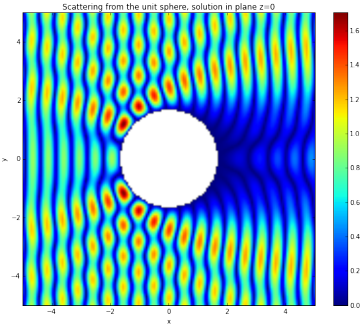
Qty of interest: $\mathrm{Vol}\{f_{pl} = 0\}$.

Examples of uncertain parameters in applications

4) Acoustic scattering of objects having uncertain shape

$$\begin{cases} \Delta u + k^2 u = 0 & \text{in } \mathbb{R}^3 \setminus D \\ \dfrac{\partial u}{\partial n} - \mathrm{i} k u = g & \text{on } \Gamma := \partial D \end{cases}$$

u : pressure, k : wave number



Uncertain shape:

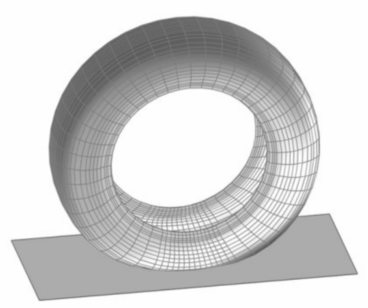
$$\Gamma = \Gamma(\omega)$$

Qty of interest:

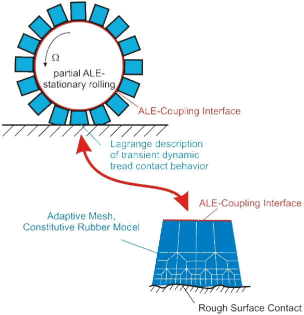
$$U_0(\omega) = u(\mathbf{x}, \omega).$$

(Source: BEM++, T. Betcke et al., www.bempp.org)

5) Rolling tire on the road: Contact with rough surfaces



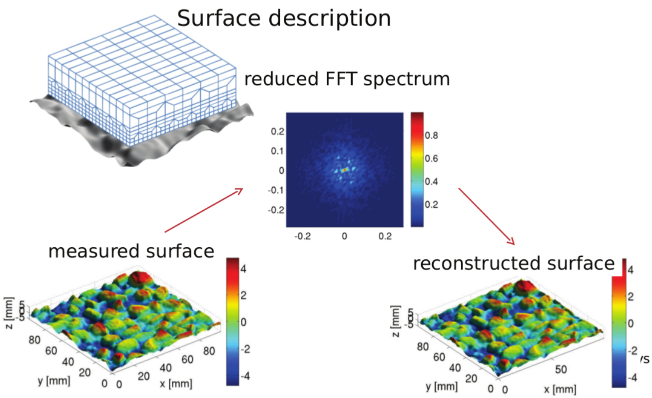
$\psi(x)$



Courtesy: Prof. Udo Nackenhorst, IBNM, Univ. Hannover

Input parameter: $\psi(x)$ is the road surface profile.
(irregular microstructure)

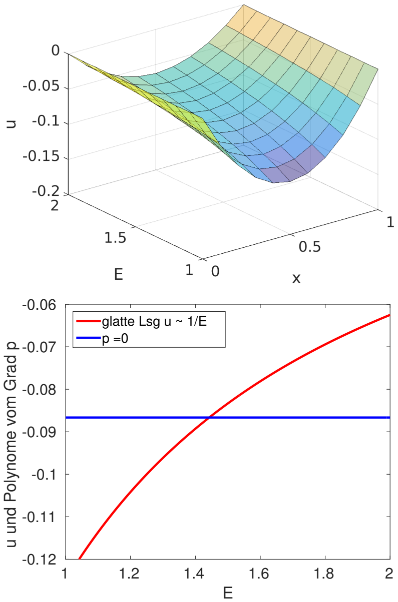
Rough Surface Contact



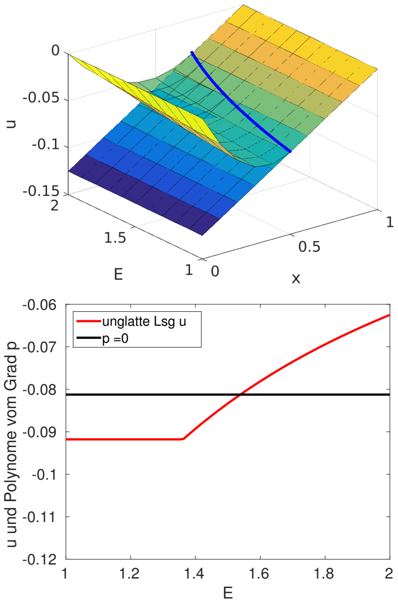
- The road surface $\psi(x)$ has an irregular microstructure;
- The actual contact zone is a union of a few spots;
- The local microstructure changes as the tire rolls.

Approximation with Polynomials

Free wire rope



Wire rope with an obstacle



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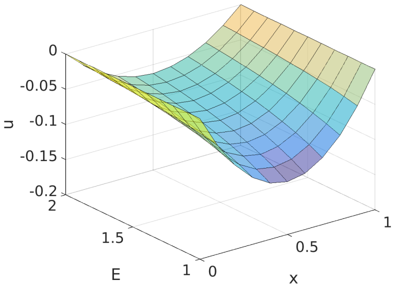

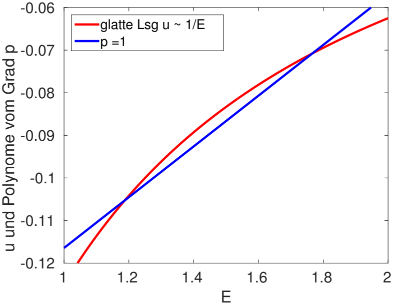

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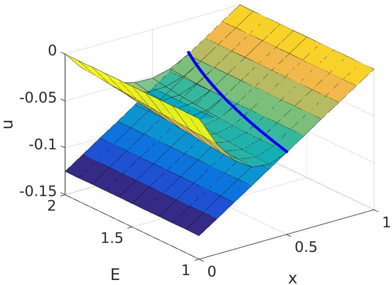

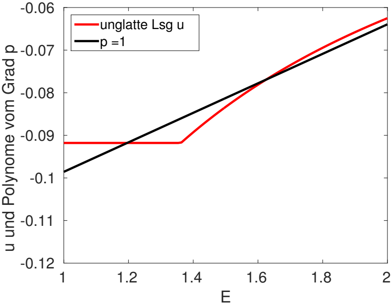

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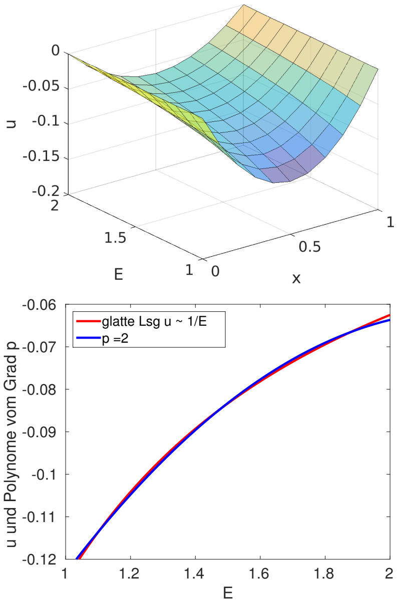

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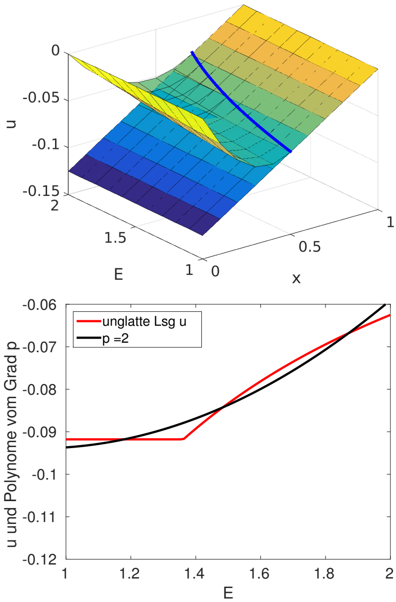

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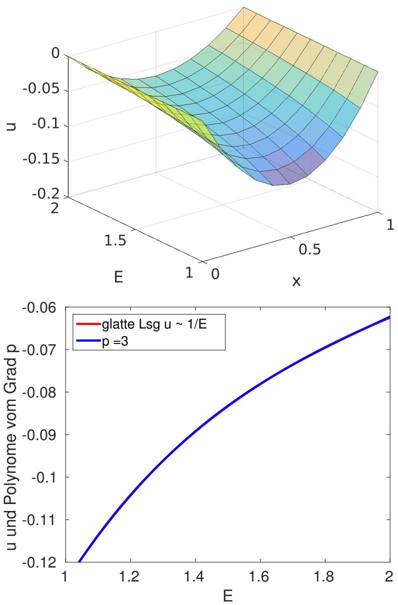

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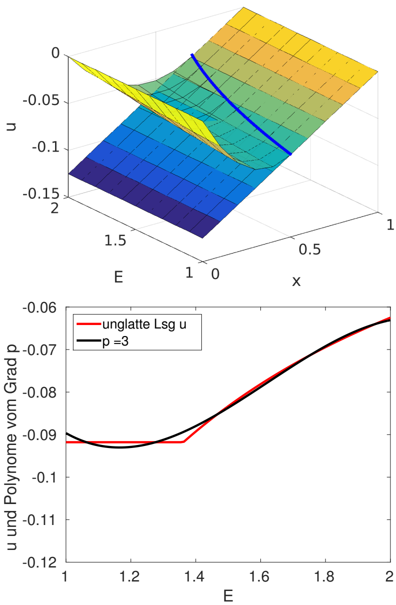

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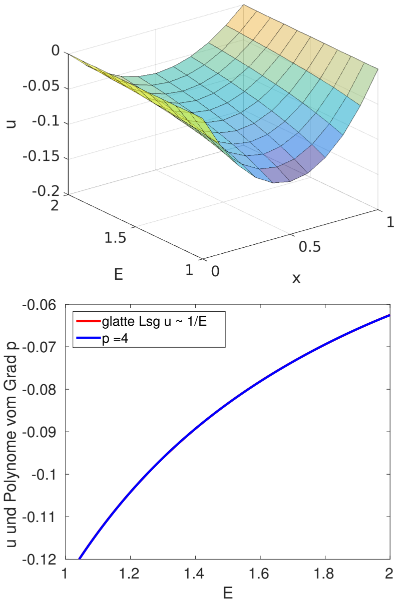

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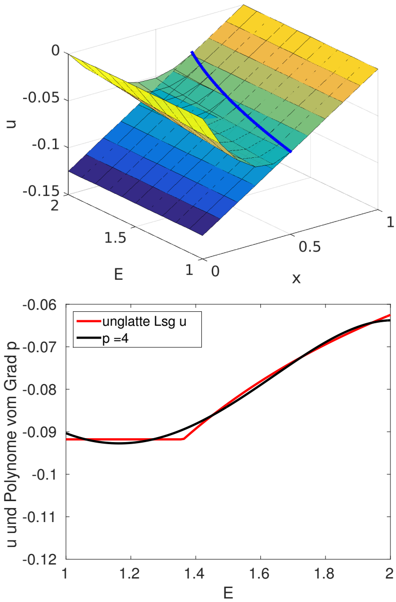

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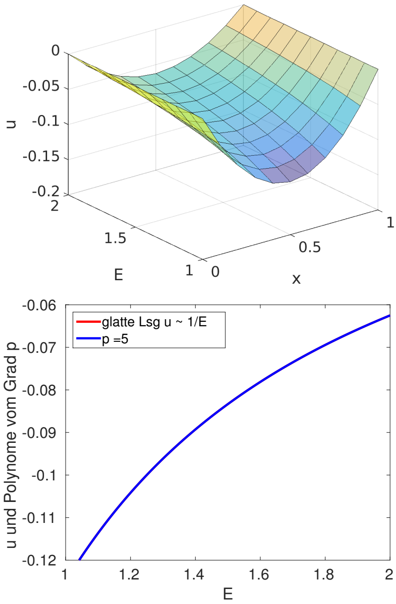

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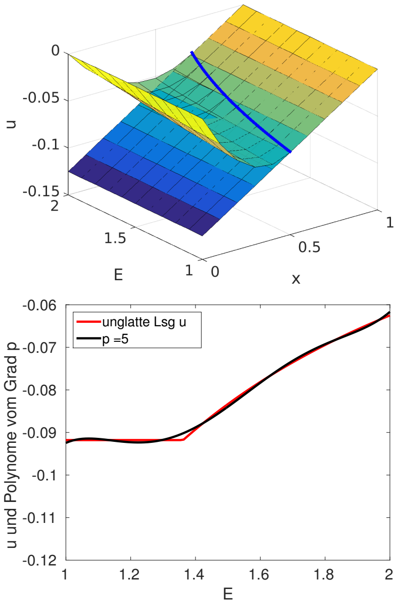

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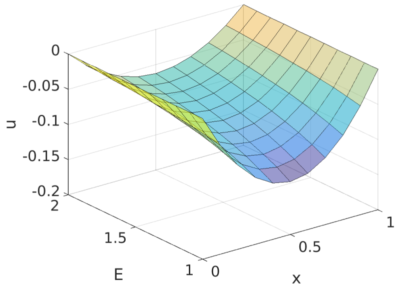

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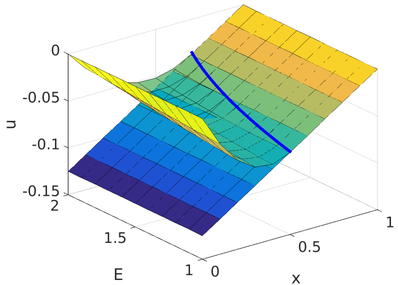

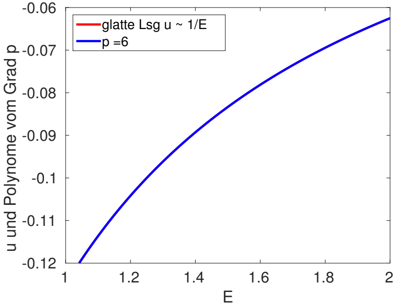

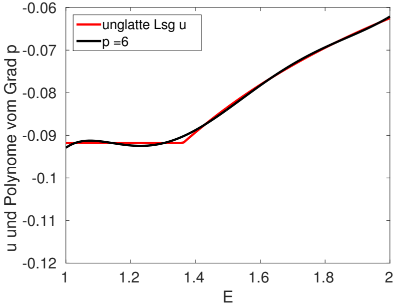

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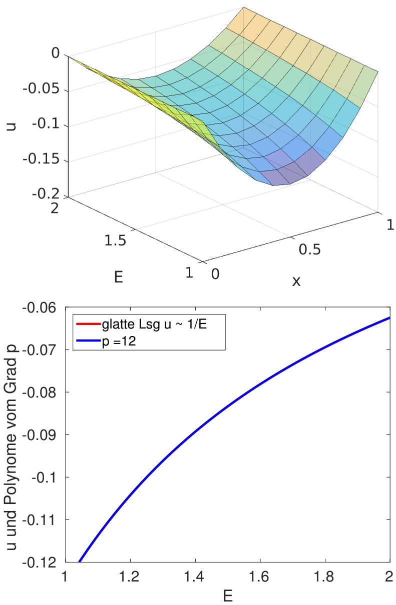

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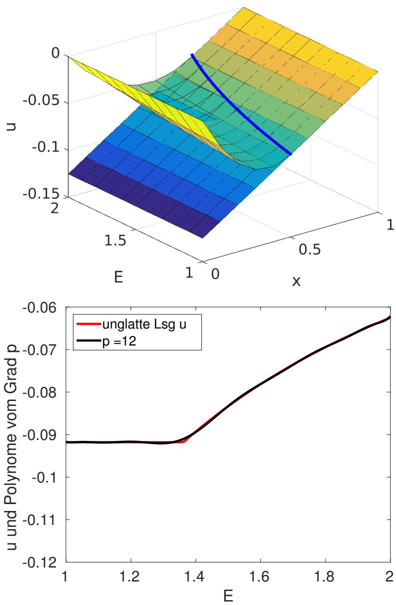

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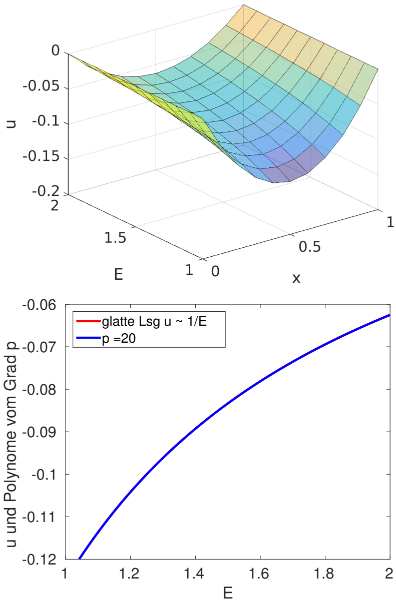

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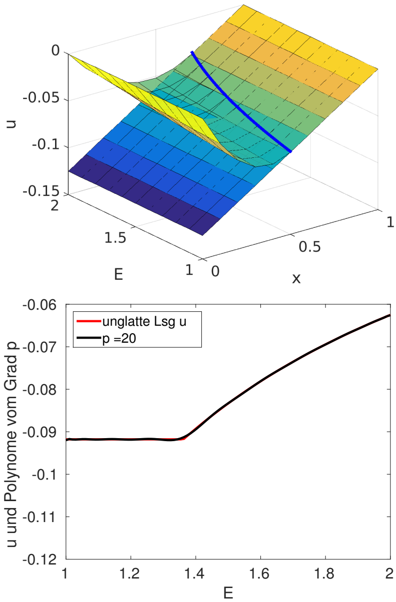
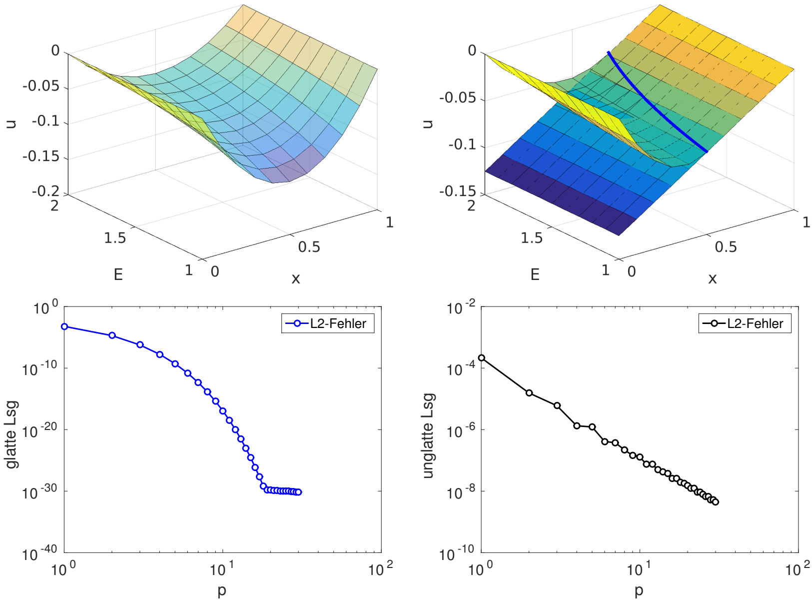
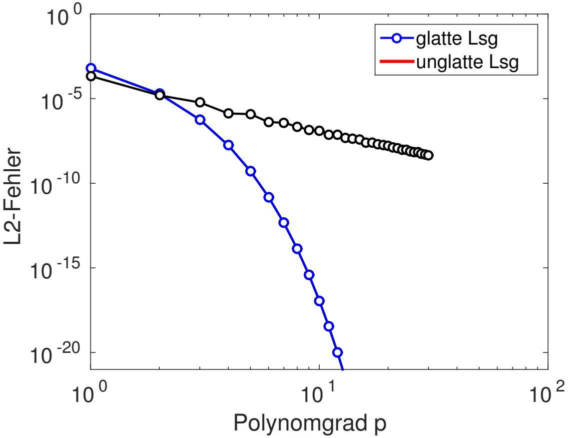


Approximation with Polynomials

Free wire rope | Wire rope with an obstacle



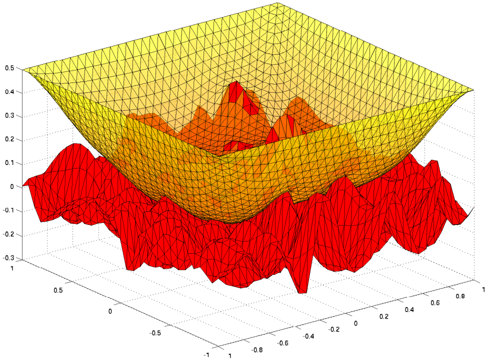
Approximation with Polynomials



Example: Contact of an elastic membrane with a rough surface (2d)

$$\left.\begin{array}{c} -\Delta u \geq f, \quad u \geq \psi, \\ (\Delta u + f)(u - \psi) = 0, \end{array}\right\} \quad \text{in } D,$$

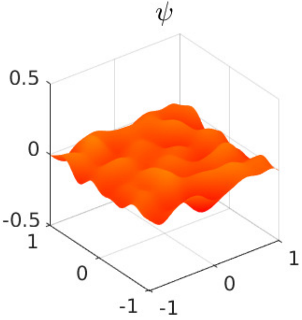
$$u = 0 \qquad \text{on } \partial D.$$



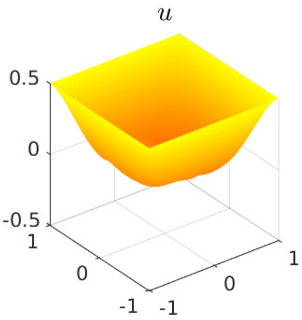
$$\left(\begin{array}{c} \text{here} \\ D = [-1, 1]^2 \end{array} \right)$$

QoI: Deformation $u(x, \omega)$; Contact Area $\Lambda(\omega) = \{x : u(x, \omega) = \psi(x, \omega)\}$.

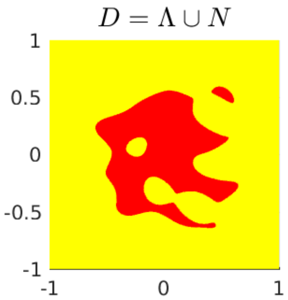
One realization of the obstacle surface $\psi = \psi(x)$:



Obstacle surface

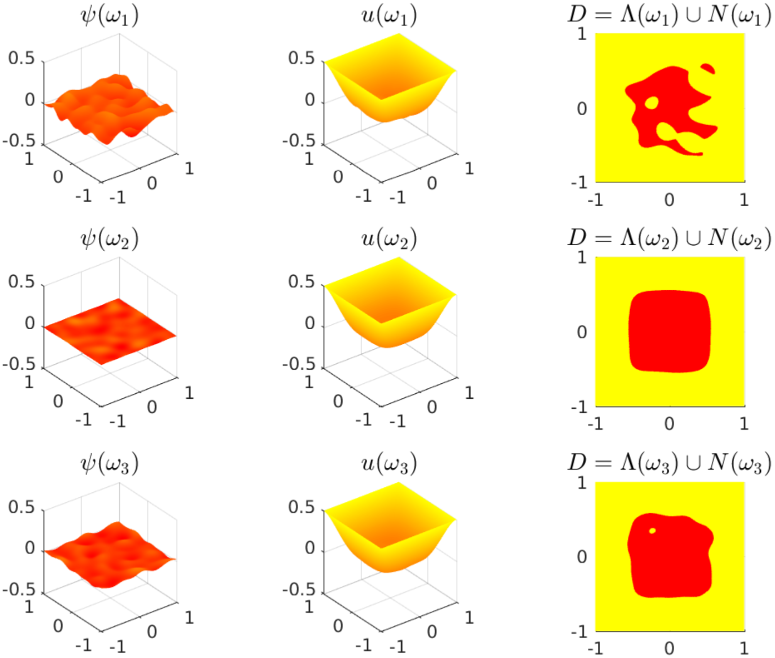


Deformation



Contact set

Obstacle surfaces of variable/random roughness $\psi = \psi(x, \omega)$:

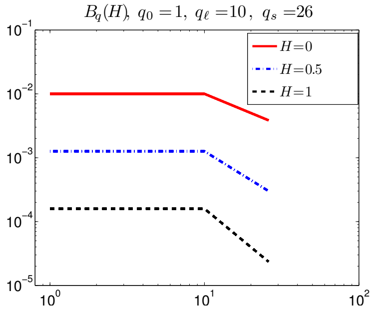


Example: Rough obstacle models

Power spectrum [Persson et al.'05]:

$$\psi(x) = \sum_{q_0 \le |q| \le q_s} B_q(H) \cos(q \cdot x + \varphi_q)$$

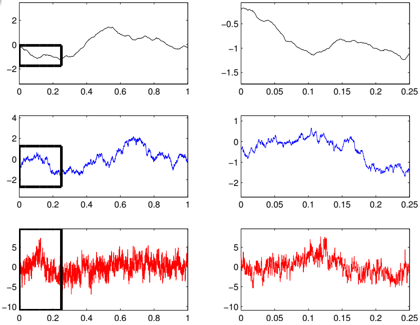
where $B_q(H) = \frac{\pi}{5}(2\pi \max(|q|, q_l))^{-H-1} \rightarrow$



Many materials in Nature and technics obey this law for amplitudes.

$H \sim \mathcal{U}(0,1)$ random roughness

$\varphi_q \sim \mathcal{U}(0, 2\pi)$ random phase

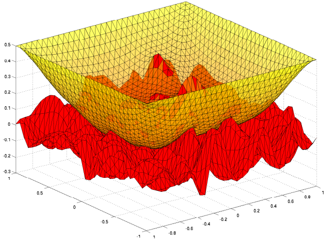


Forward solver:

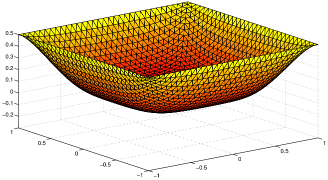
Own implementation of MMG (TNNM)

[Kornhuber'94,...]

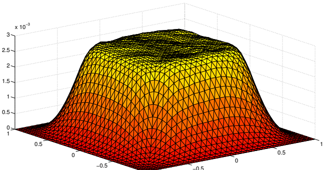
Approximation of $\mathbb{E}[u]$ and $\mathrm{Var}[u]$ of the deform. field $u(x, \omega)$



A realization of the obstacle $\psi^i(x)$ and the deformation profile $u_h^i(x)$

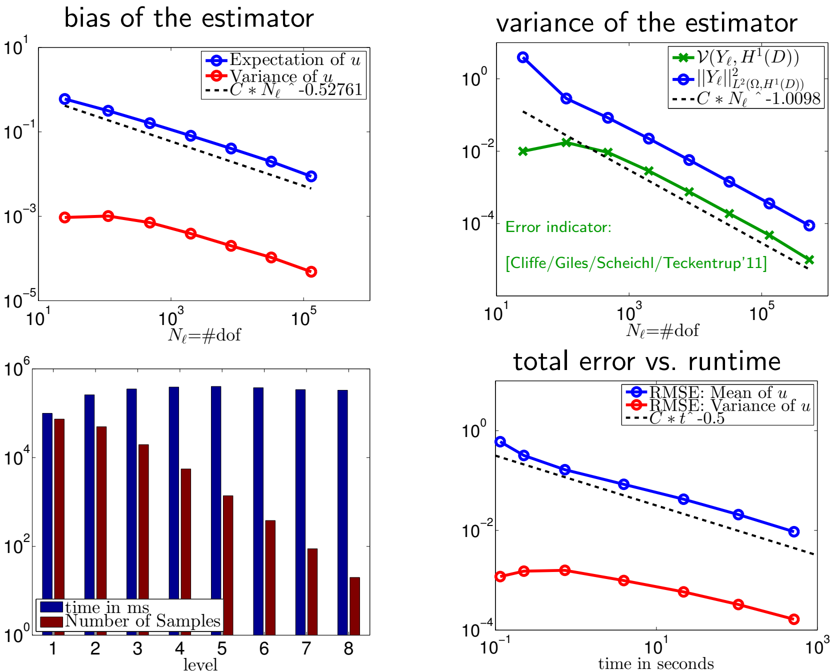


The mean deformation profile $E^{ML}[u]$

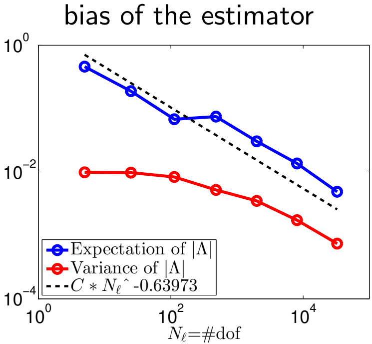


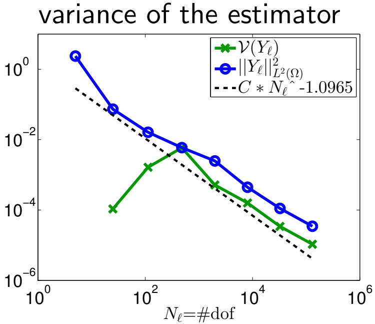
The variance of the deformation profile $V^{ML}[u]$

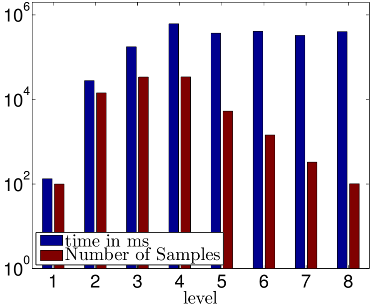
Approximation of $\mathbb{E}[u]$ and $\mathrm{Var}[u]$ of the deform. field $u(x,\omega)$

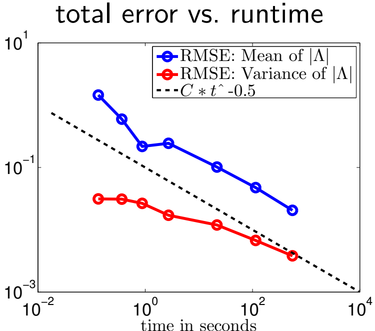


Approximation of $\mathbb{E}[X]$ and $\mathrm{Var}[X]$ of the contact area $X = |\Lambda|$









Estimators for the Variance:

Recall the mean estimator

$$E^{ML}[X] := \sum_{\ell=1}^{L} E_{M_\ell}[X_\ell - X_{\ell-1}]$$

where $$E_M[X_\ell] := \frac{1}{M}\sum_{i=1}^{M} X_\ell^i.$$

Benefits:

- $V^{ML}[X]$ is unbiased, i.e. $\mathbb{E}\left[V^{ML}[X] - \mathbb{V}[X_L]\right] = 0$
- Fast one pass stable evaluation formulae (single level in [Pebay'08])

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see Bierig, Chernov, Numer. Math. (2015)

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Theorem (a priori estim.: random obstacle problem, [Bierig/AC'15])

Suppose: $\psi \in L^\infty(\Omega, W^{2,r})$ for some $r > 2$

Deterministic fwd solver: $\|u_\ell - u\|_{H^1} \lesssim h_\ell$, pw. lin. FE

with the Total Work $\sim \ell^\nu N_\ell$ $\quad (N_\ell \sim h_\ell^{-2}$, i.e. lin. cost).

Then: MLMC with the optimal choice $M_\ell := (h_\ell / h_L)^2$ satisfies

$$\left.\begin{aligned} \|E^{ML}[u] - \mathbb{E}[u]\|_{L^2(\Omega,H^1)} \\ \|V^{ML}[u] - \mathbb{V}[u]\|_{L^2(\Omega,H^1)} \end{aligned}\right\} \lesssim h_L \sqrt{|\log h_L|},$$

with the Total Work $\sim L^{\nu+1} N_L$.

Almost linear complexity for MLMC + MMG.

(Sampling is asymptotically almost for free!)

Theorem (a priori estim.: random obstacle problem, [Bierig/AC'15])

Suppose: $\psi \in L^{2q}(\Omega, W^{2,2})$ and $\frac{1}{p} + \frac{1}{q} = 1$

Deterministic fwd solver: $\|u_\ell - u\|_{H^1} \lesssim h_\ell$, pw. lin. FE

with the Total Work $\sim \ell^\nu N_\ell$ $\quad (N_\ell \sim h_\ell^{-2}$, i.e. lin. cost).

Then: MLMC with the optimal choice $M_\ell := (h_\ell / h_L)^2$ satisfies

$$\|E^{ML}[u] - \mathbb{E}[u]\|_{L^2(\Omega, H^1)} \lesssim h_L \sqrt{|\log h_L|},$$

$$\|V^{ML}[u] - \mathbb{V}[u]\|_{L^2(\Omega, H^1)} \lesssim h_L^{\frac{1}{p}}, \qquad \text{(using inv. ineq.)}$$

with the Total Work $\sim L^{\nu+1} N_L$.

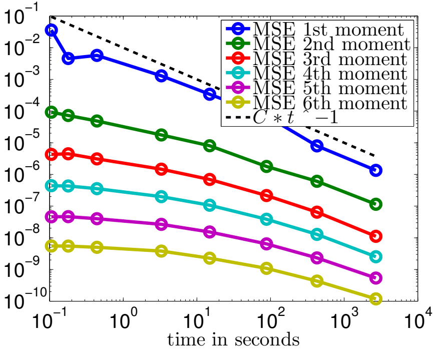
Almost linear complexity for MLMC + MMG.

(Sampling is asymptotically almost for free!)

Extension to higher order moments: $\mathcal{M}^k[X] := \mathbb{E}[(X - \mathbb{E}[X])^k]$

$$S_M^3[X] := \frac{M}{(M-1)(M-2)} \sum_{i=1}^{M} (X_i - E_M[X])^3 \qquad \text{(unbiased)}$$

$$S_M^k[X] := \frac{1}{M} \sum_{i=1}^{M} (X_i - E_M[X])^k \qquad \text{(small bias)}$$

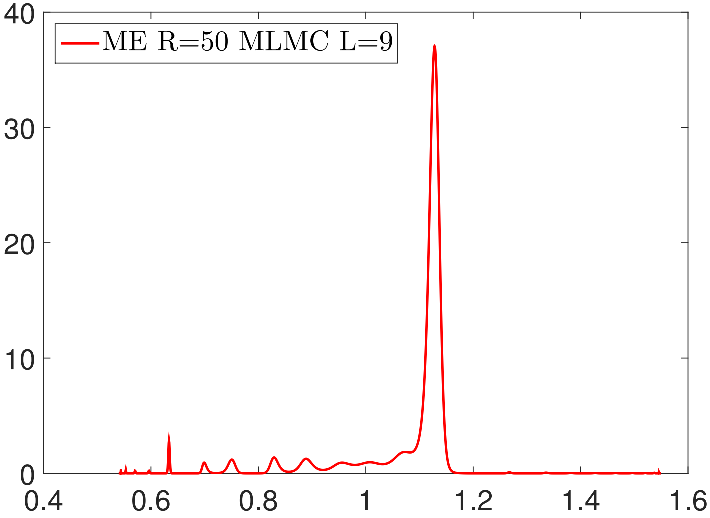


$X = |\Lambda|$, contact area

Notice:
$|\Lambda| \leq |D|$

[Bierig, Chernov, JSPDE'16]

Estimation of the PDF ρ_X of the contact area $X = |\Lambda|$ by the Maximum Entropy method



The peak(s) corresponds to ca. 28.2% of the membrane in contact with the surface

More experiments and rigorous error analysis in [Bierig/Chernov, JCP'16]

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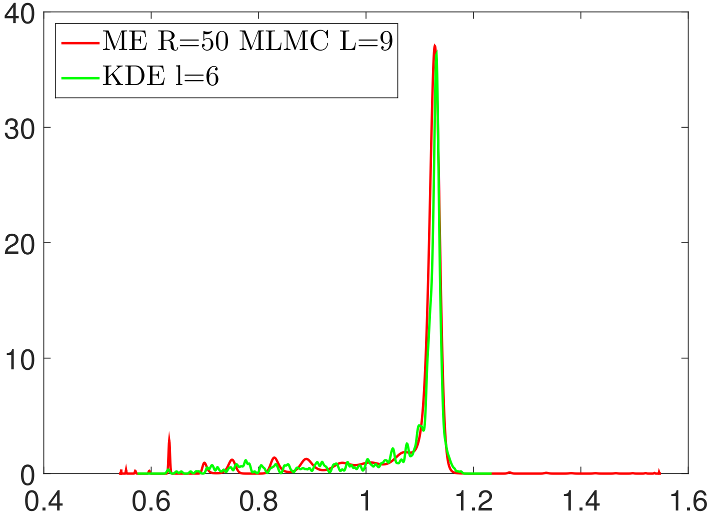

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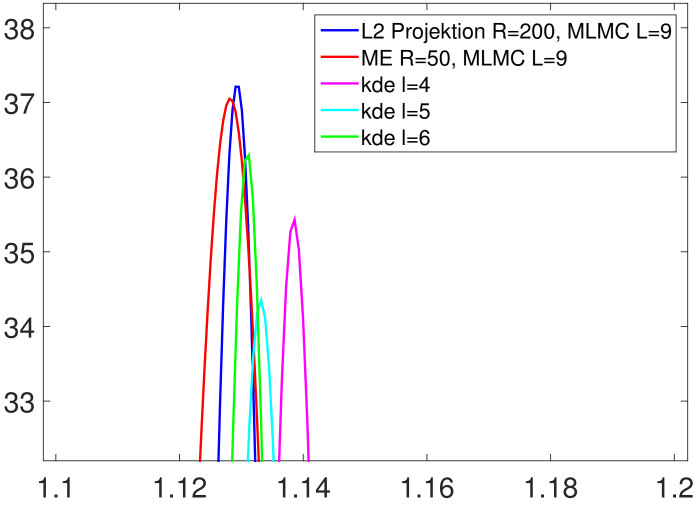

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Towards adaptivity – adaptive selection of

- the number of moments R
- the interval of approximation $[a, b]$

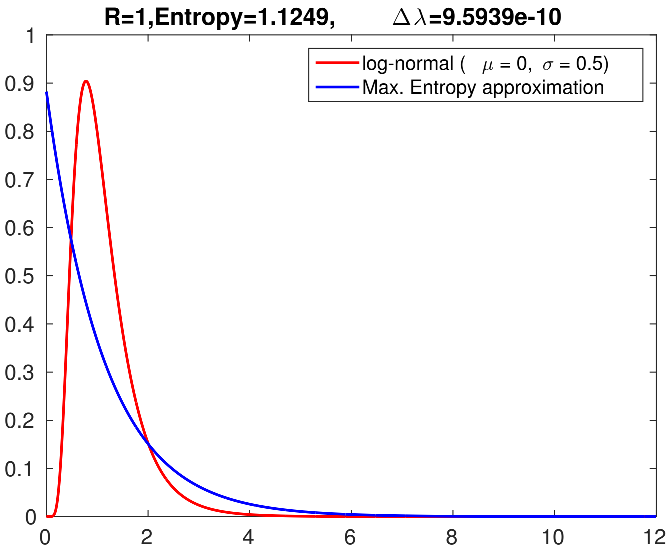
Test example:

Log-normal distribution with $\mu = 0$ and variable σ ($= 0.5$ and 0.2)

Estimation of moments $\mu_1, \ldots, \mu_R$ by MC with 10^8 samples

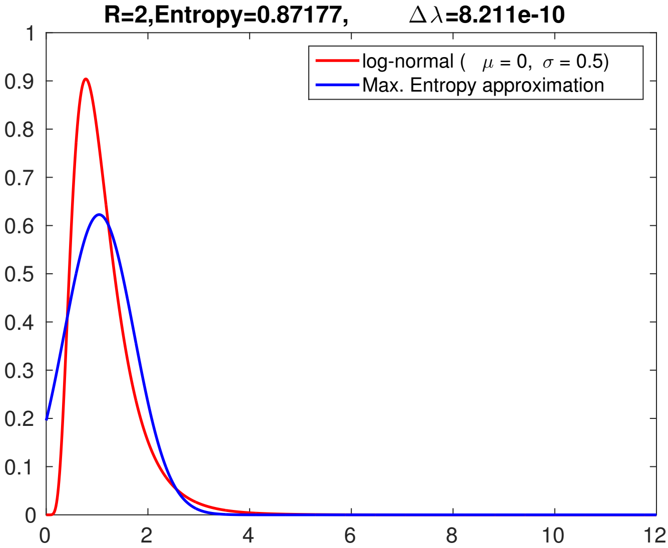
Stopping parameters for the Newton Method:

- $\Delta\lambda \leq 10^{-9}$ (convergence)
- $\Delta\lambda \geq 10^{3}$ (no convergence)
- $\#\texttt{iter} \geq 1000$ (no convergence)



Legendre Moments:

- Stable for $R \leq 8$
- Entropy is may decrease even when the Newton Method does not converge



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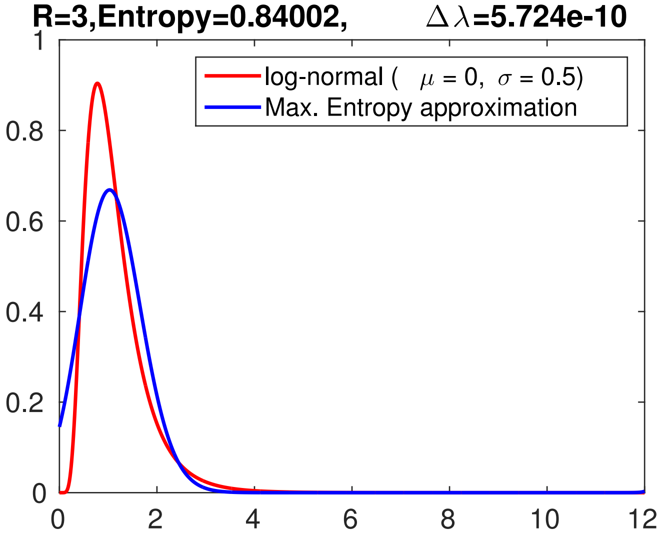

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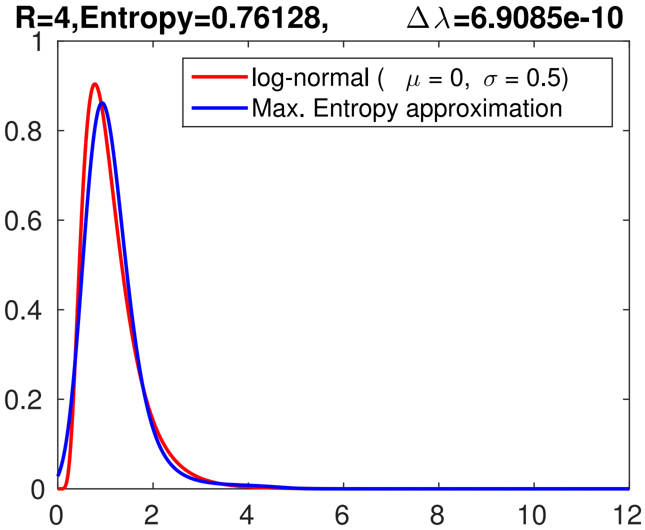

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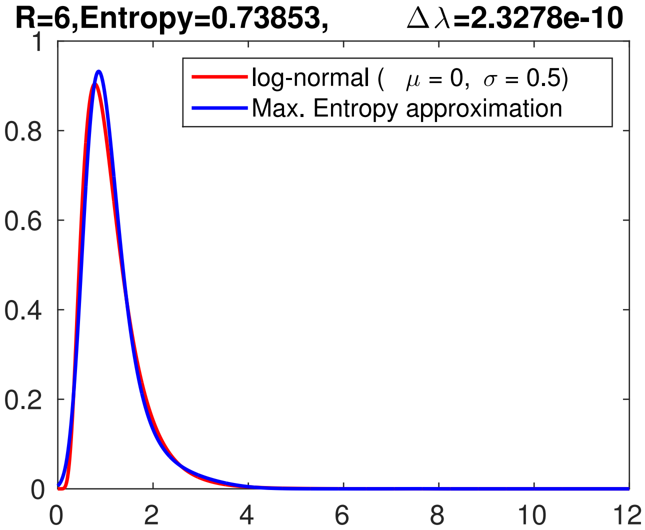

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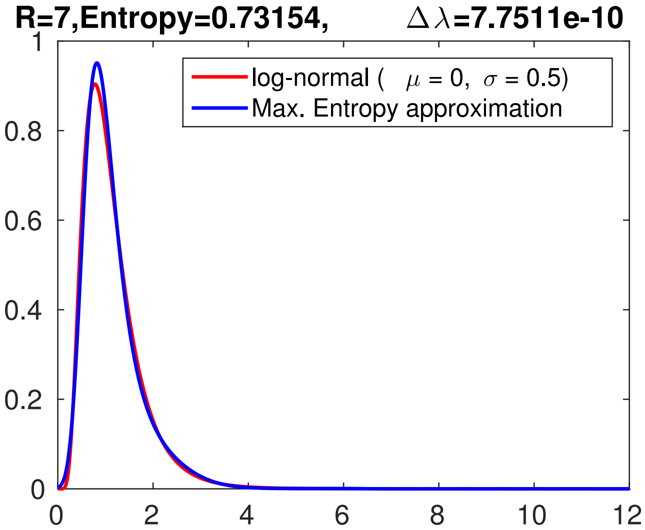

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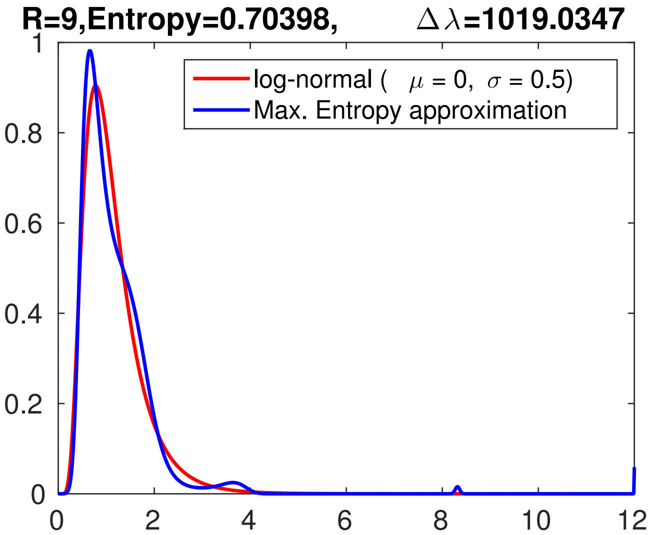

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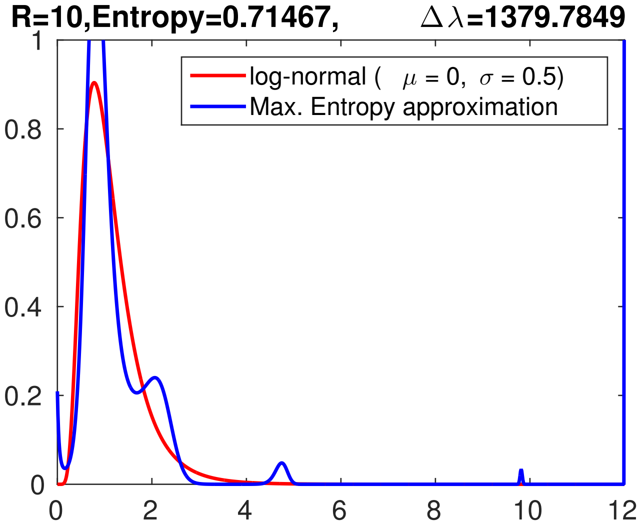

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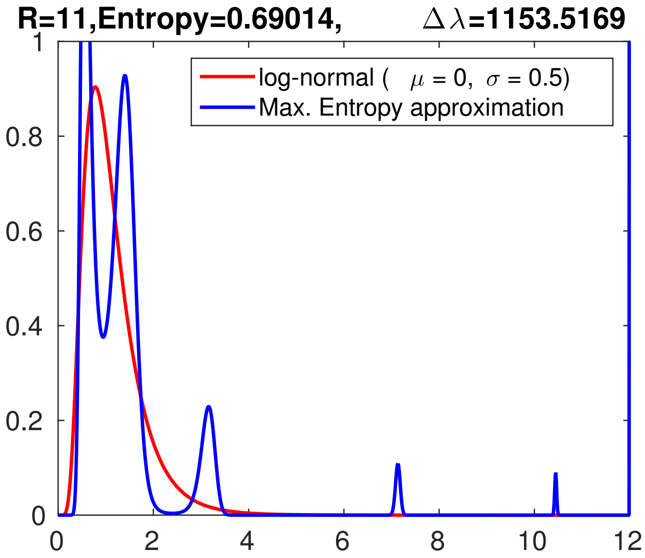

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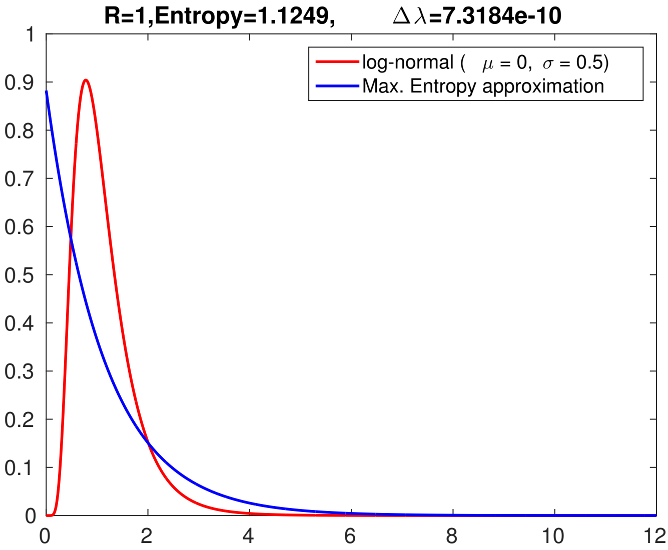

Monomial Moments:

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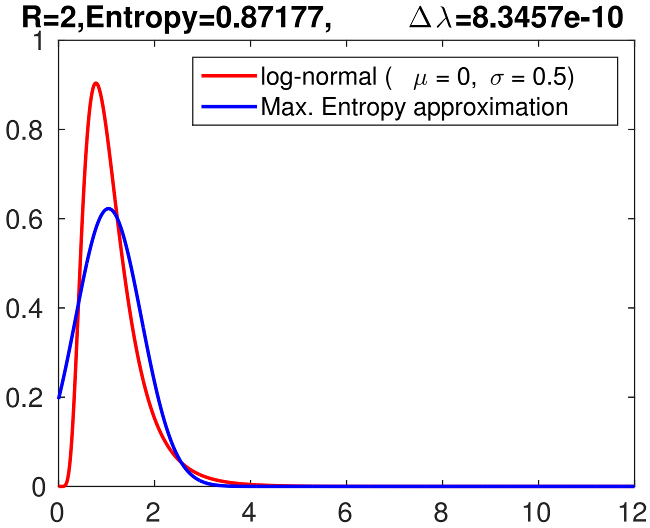

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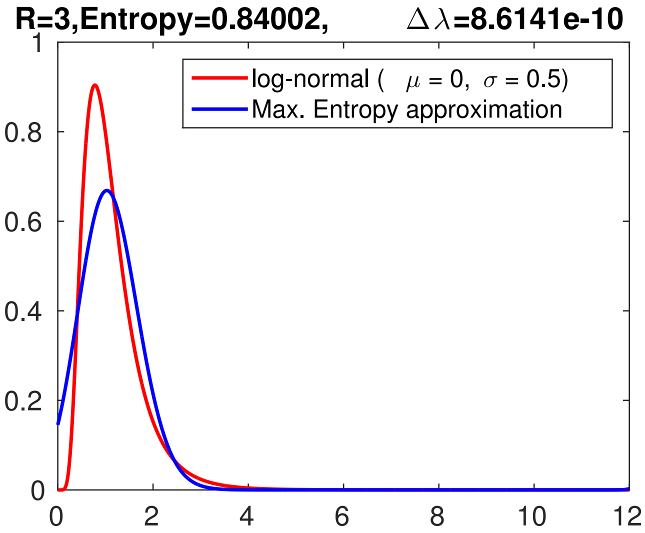

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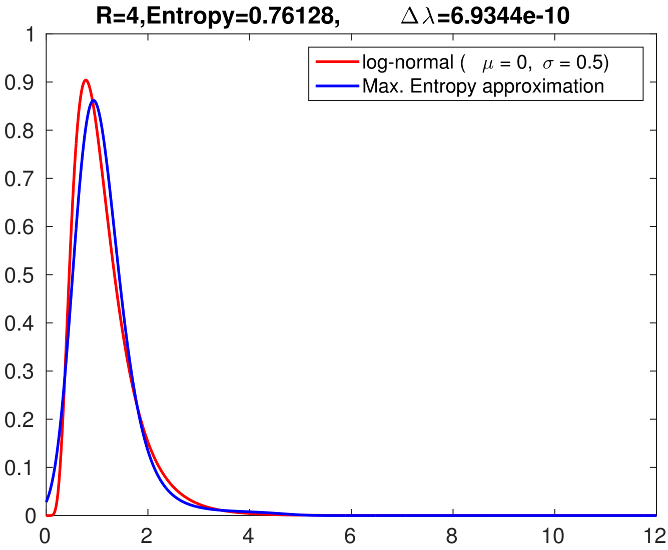

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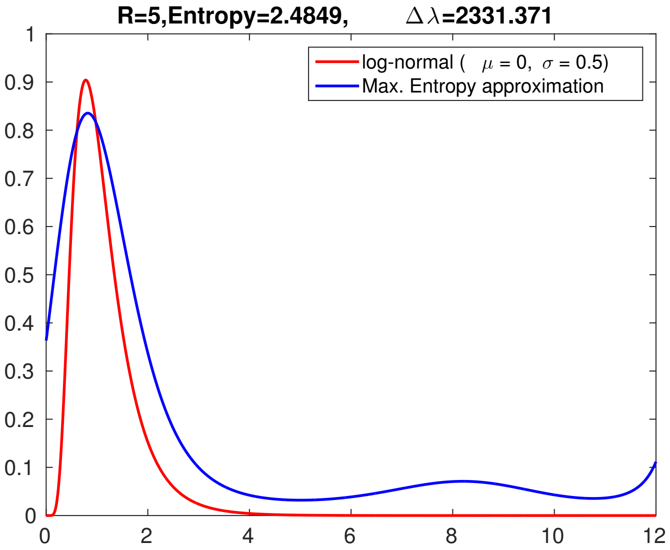

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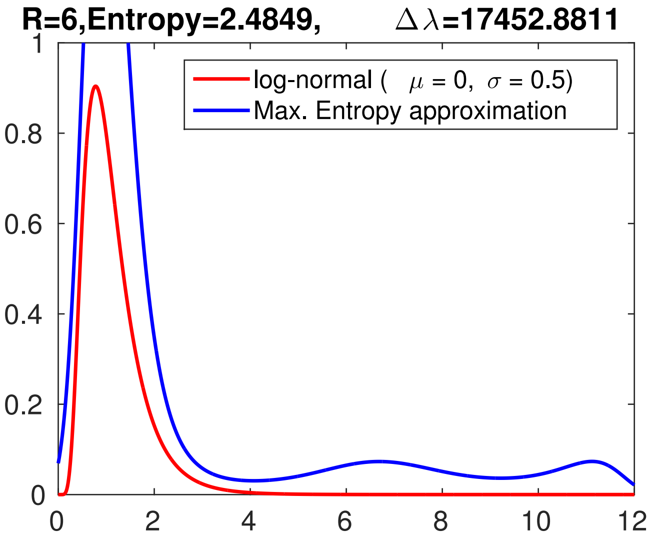

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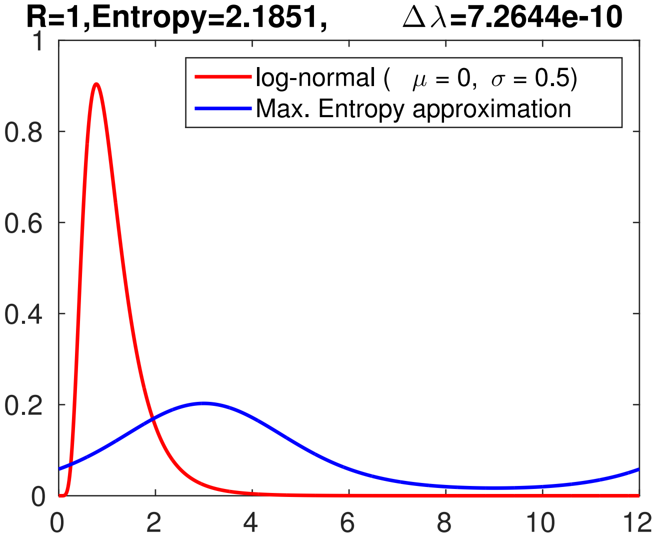
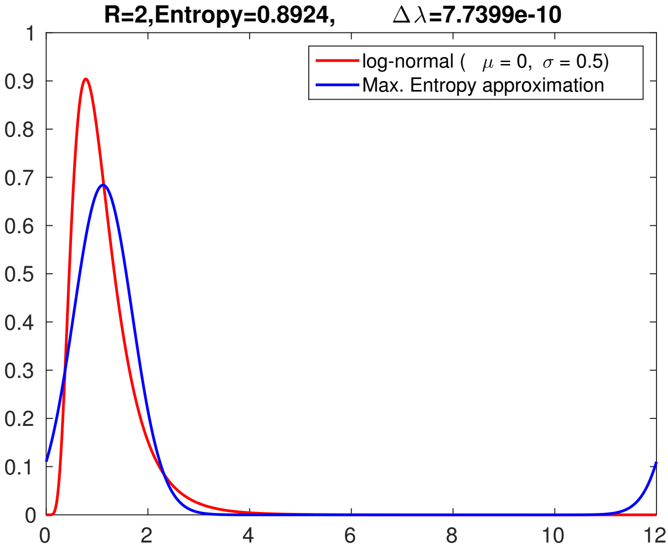


Fourier Moments:

- Stable
- Entropy is monotonously decreasing



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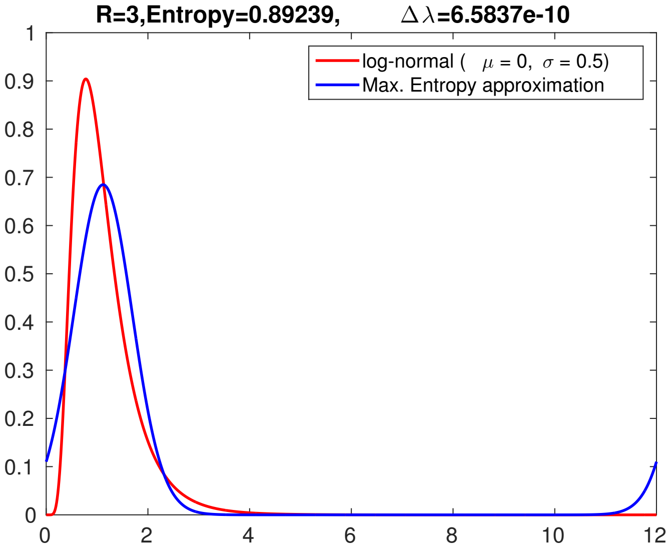

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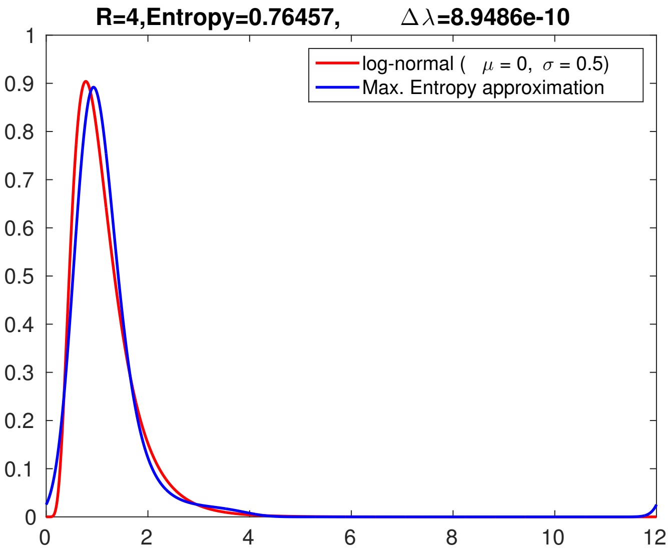

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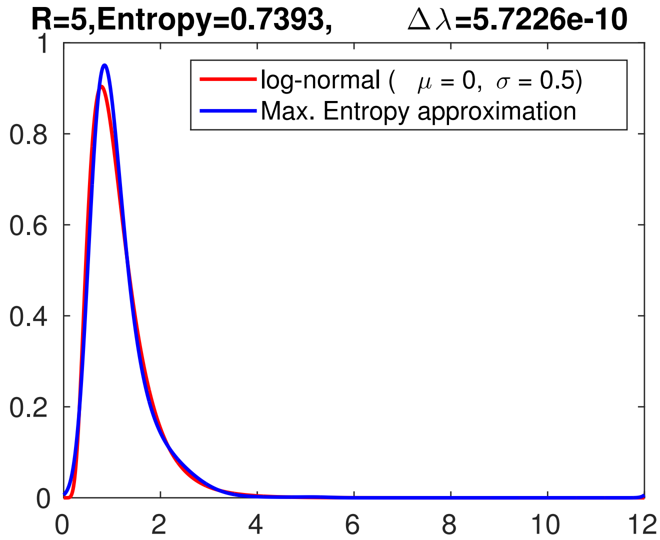

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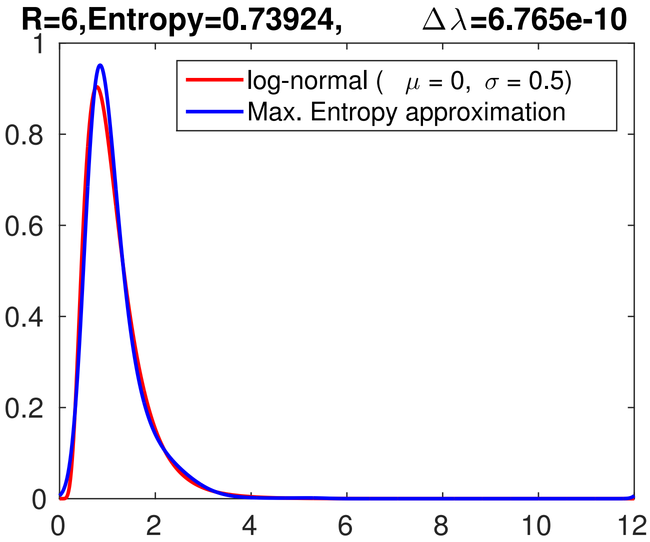

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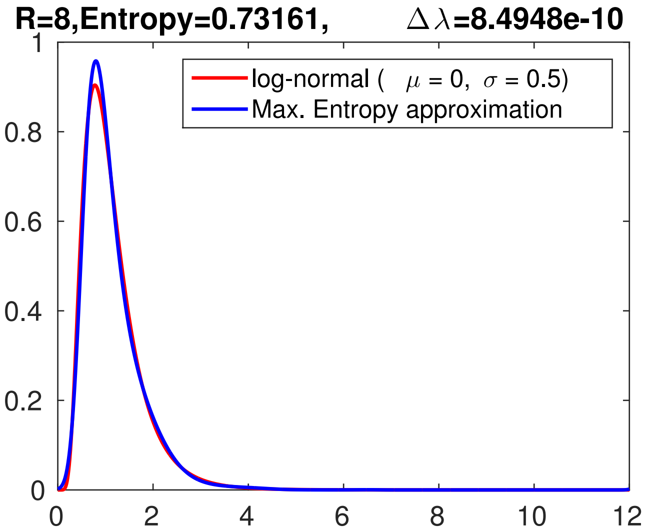

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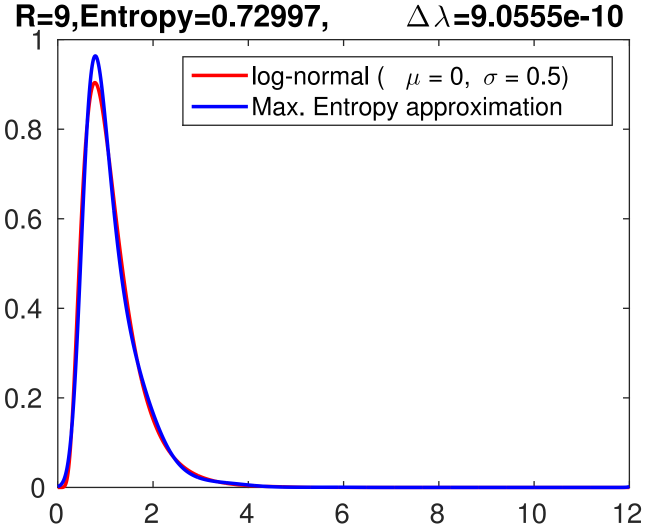

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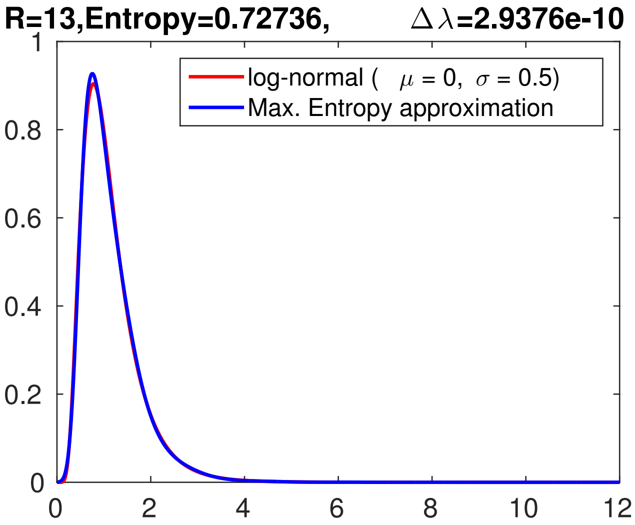

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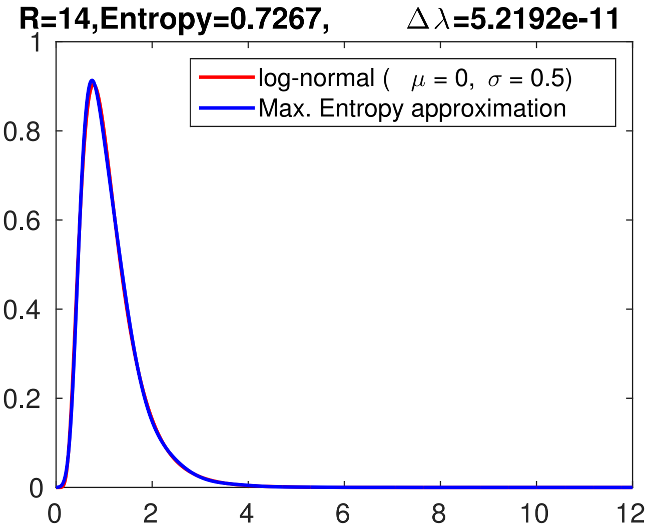

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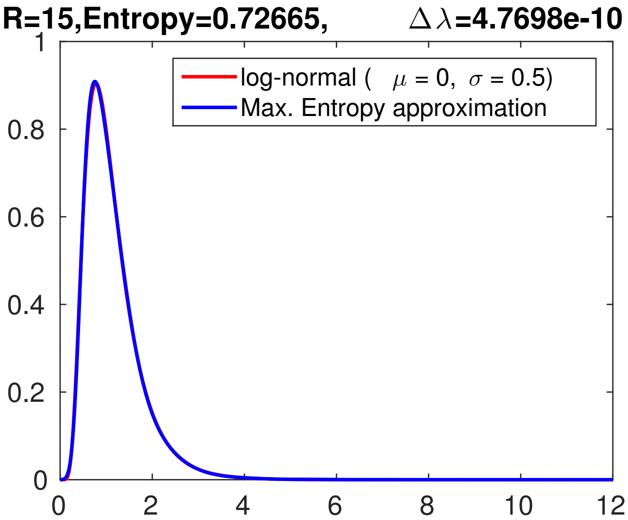

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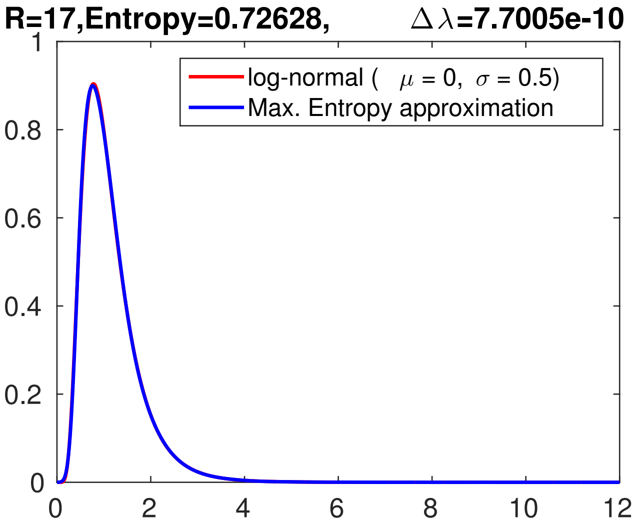

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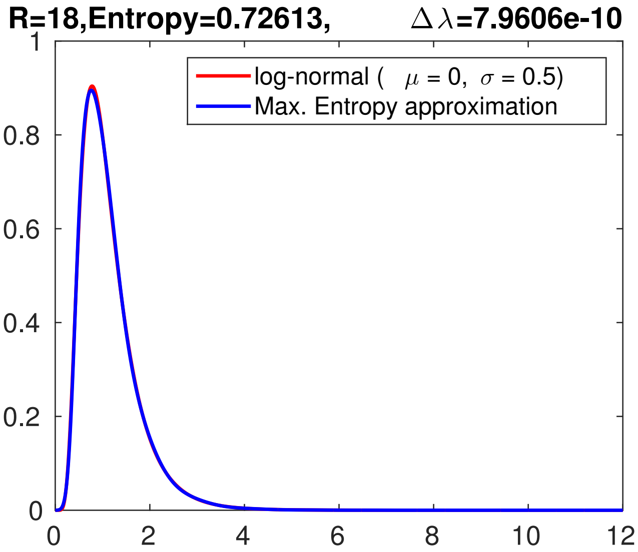
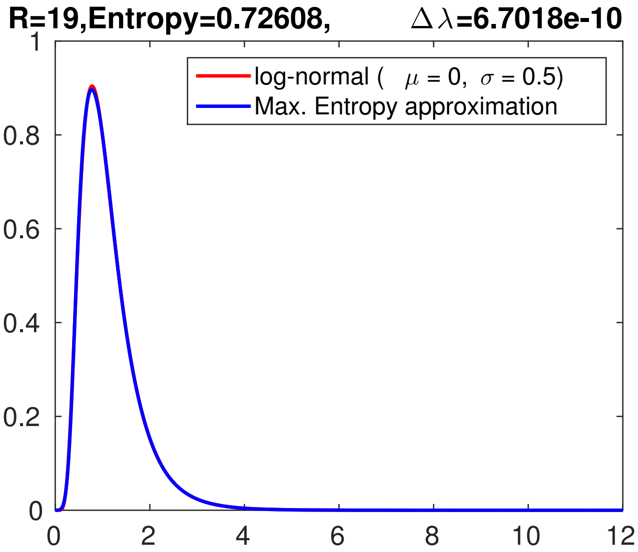
- Stable
- Entropy is monotonously decreasing



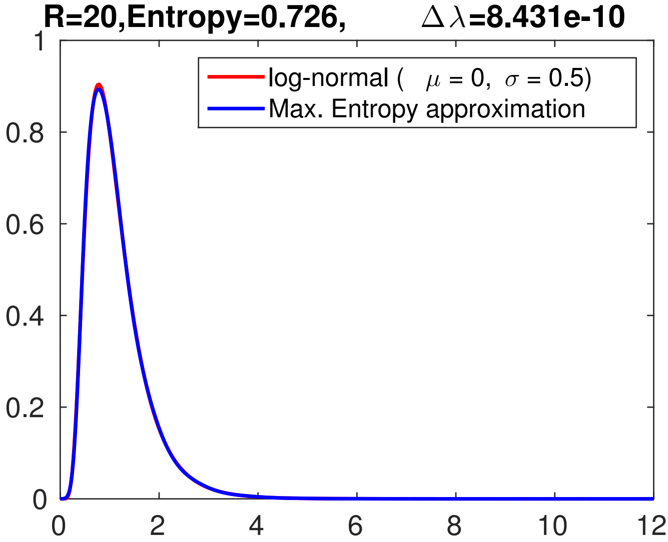
Fourier Moments:

- Stable
- Entropy is monotonously decreasing



Fourier Moments:

- Stable
- Entropy is monotonously decreasing

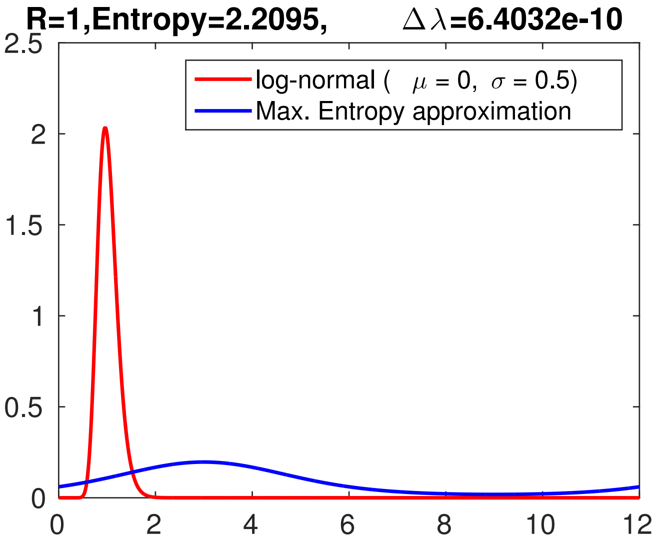


Fourier Moments:

- Stable
- Entropy is monotonously decreasing

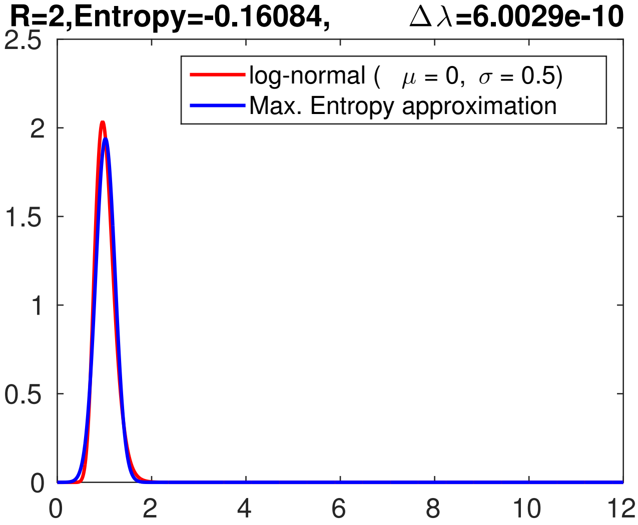
Breaking convergence for the Fourier basis by choosing a more concentrated density!

e.g. log-normal with $\mu = 0$, $\sigma = 0.2$



Fourier Moments ($\sigma = 0.2$, $[a, b] = [0, 12]$):

- Remain stable even without convergence!
- Entropy is still monotonously decreasing!



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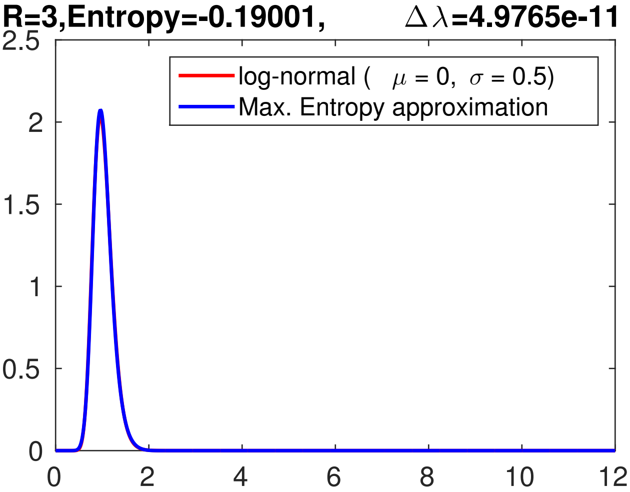

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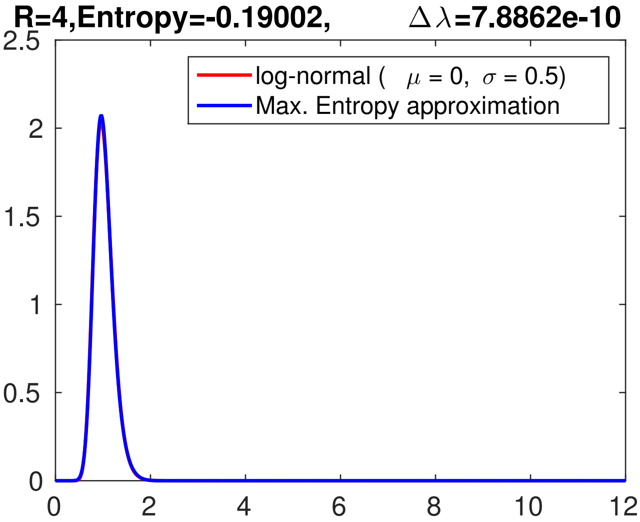

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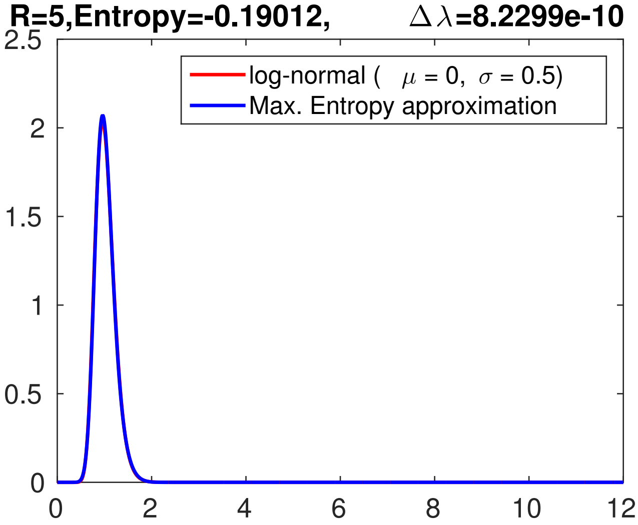

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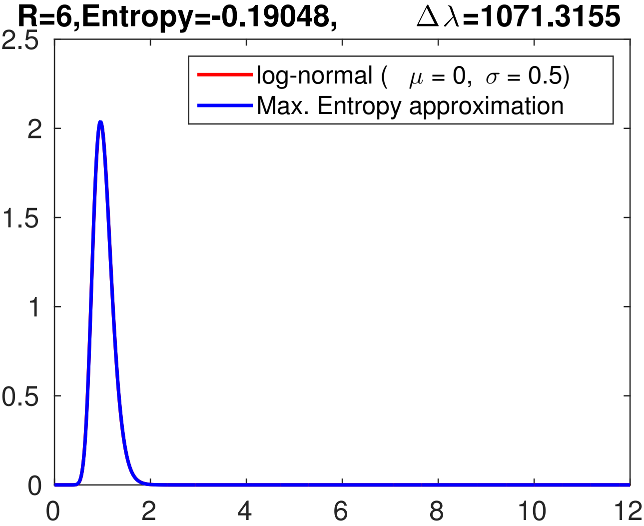

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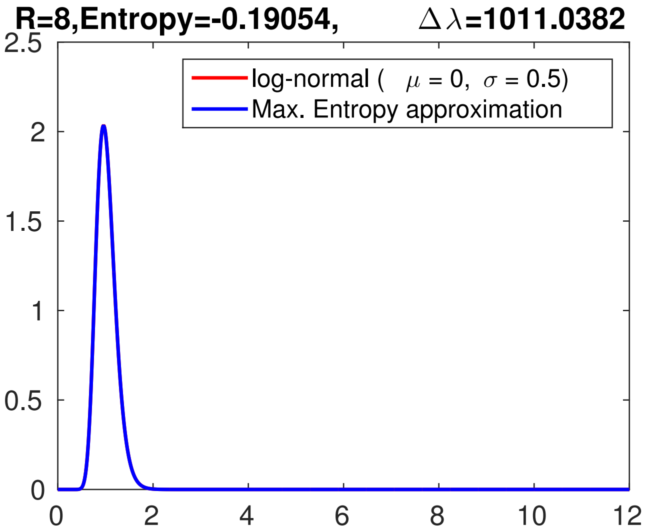

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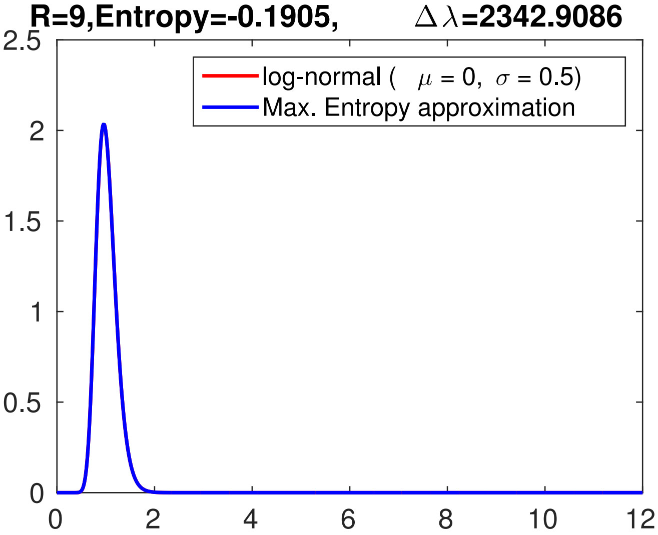

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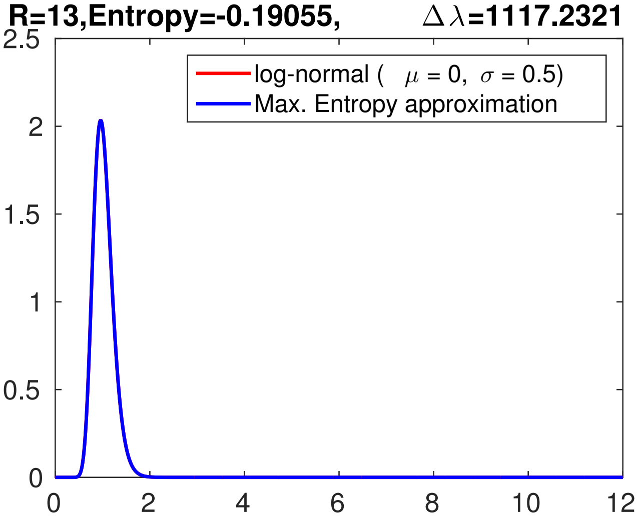

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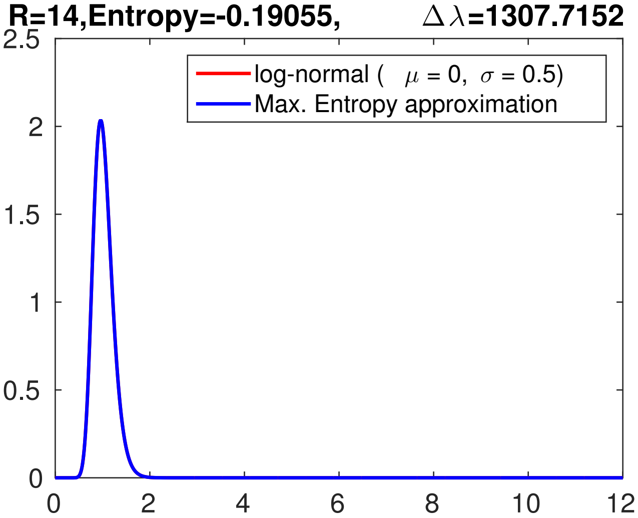

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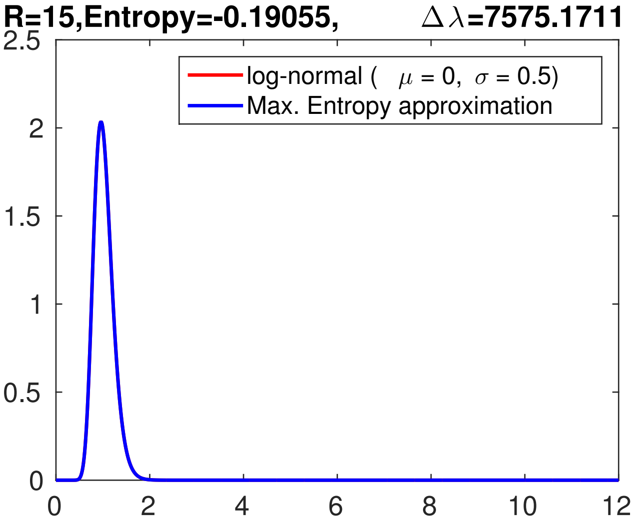

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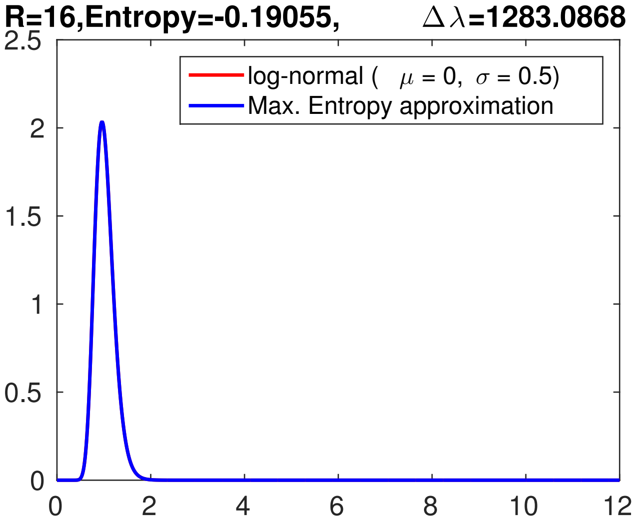
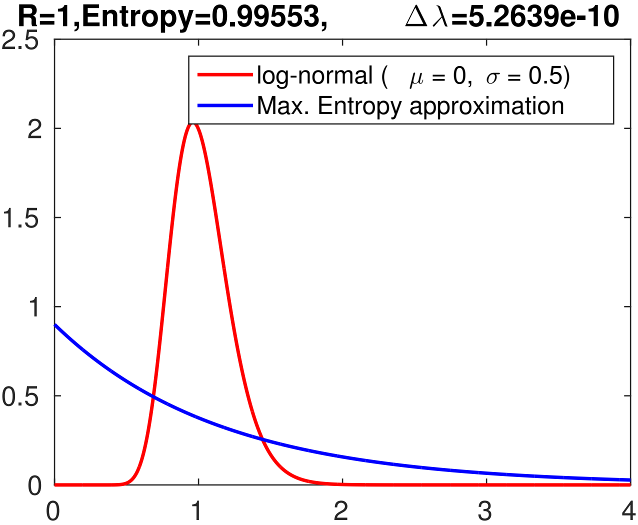


Fourier Moments ($\sigma = 0.2$, $[a, b] = [0, 12]$):

- Remain stable even without convergence!
- Entropy is still monotonously decreasing!

Regain stability of the Legendre basis
by choosing a smaller approximation interval!

e.g. $[a, b] = [0, 4]$



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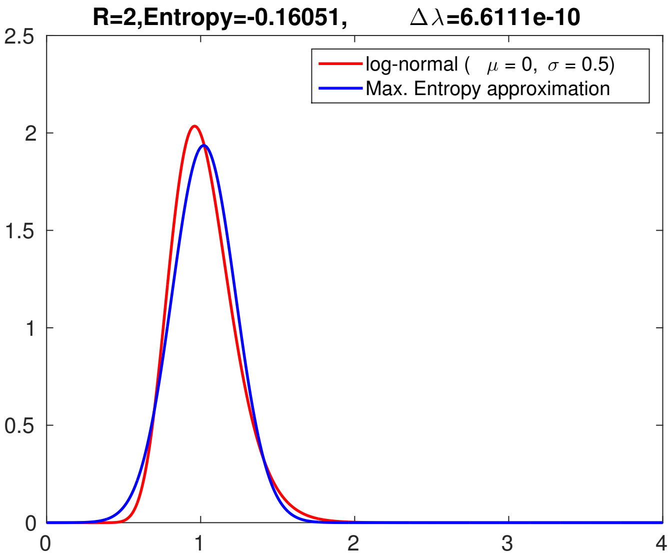
- Entropy is still monotonously decreasing!



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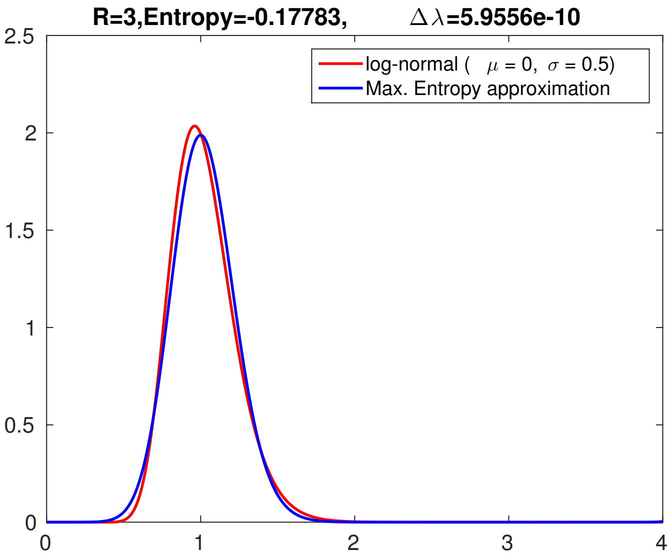

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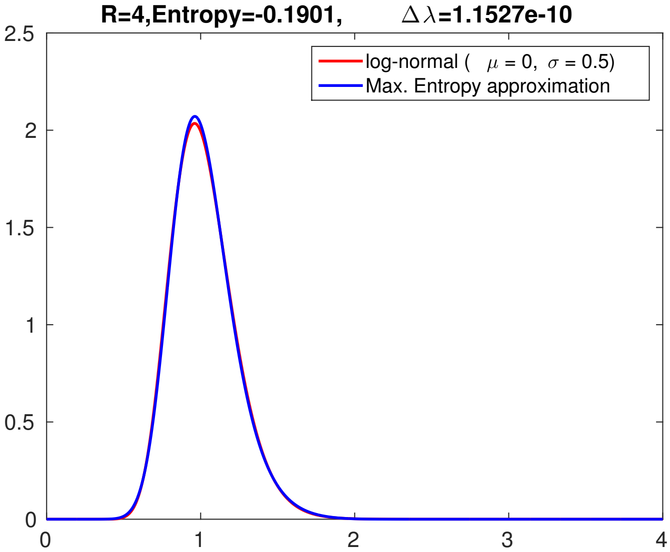

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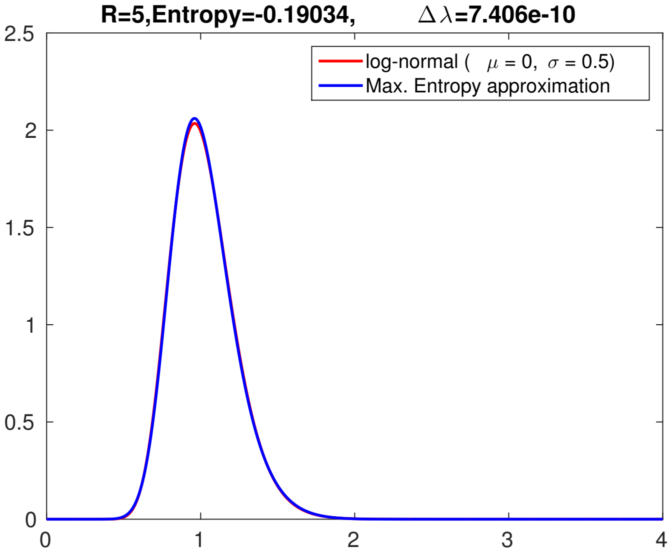

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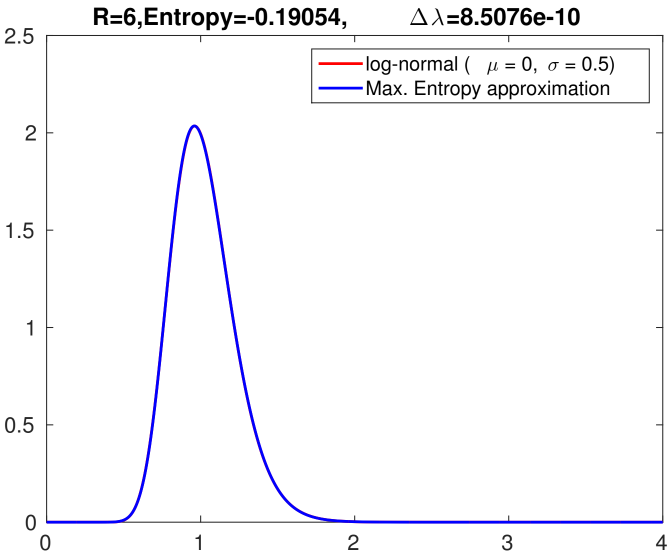

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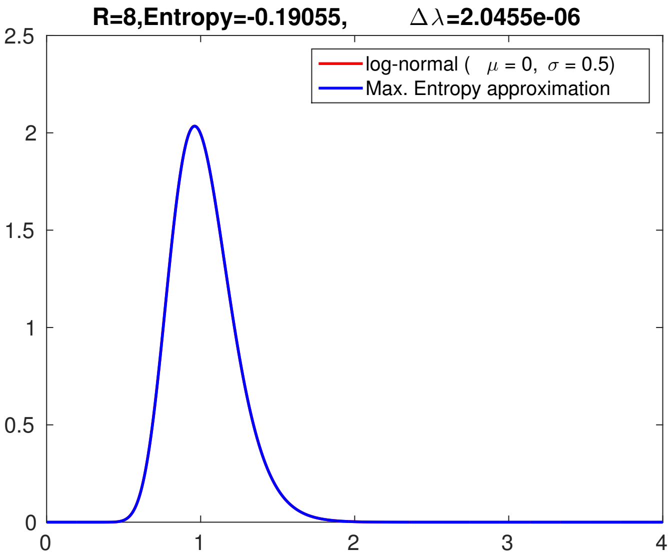

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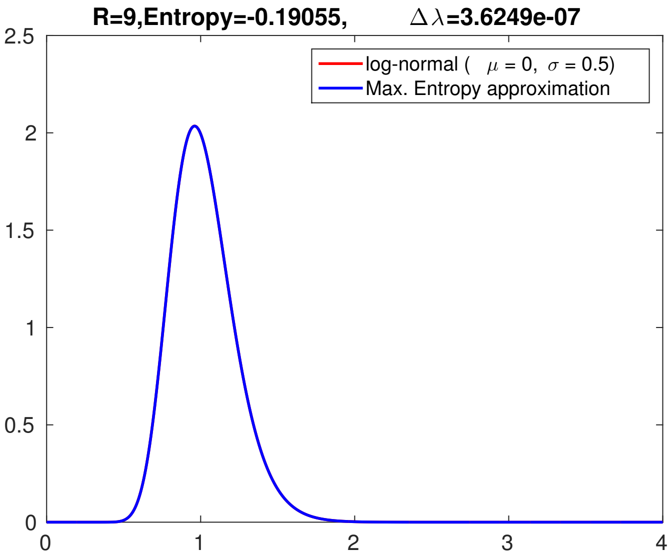

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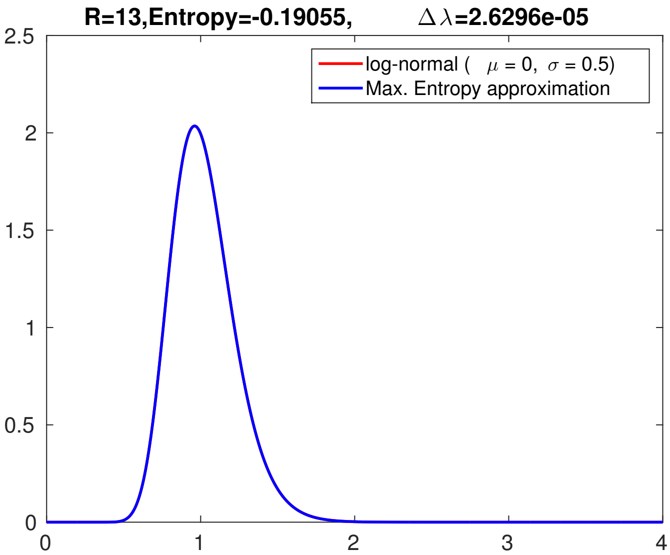

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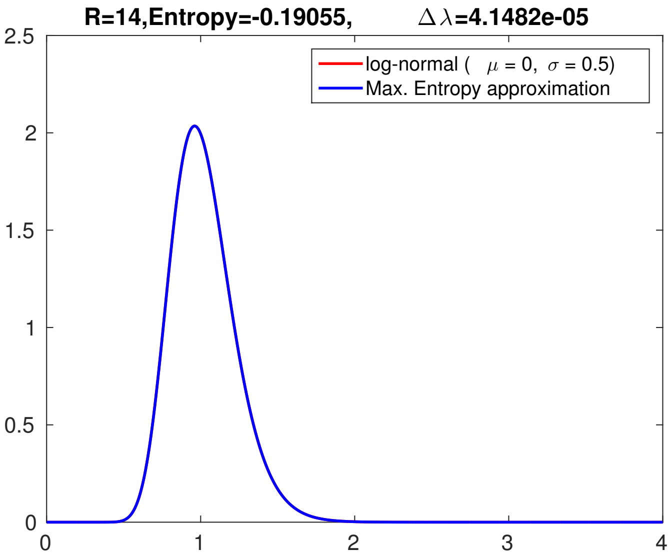

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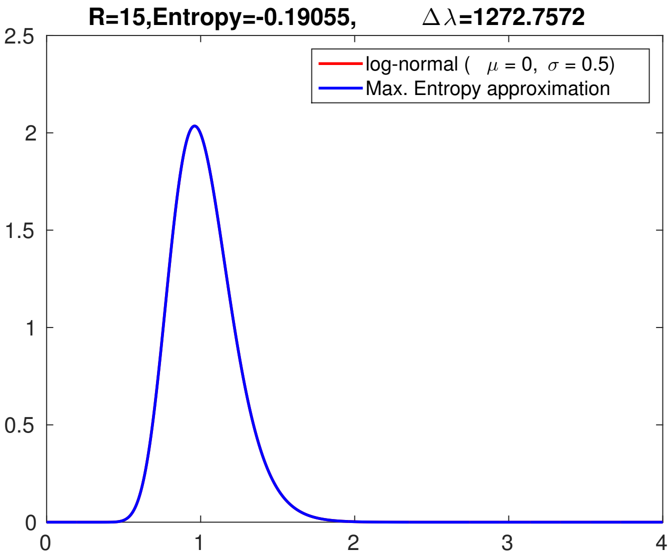

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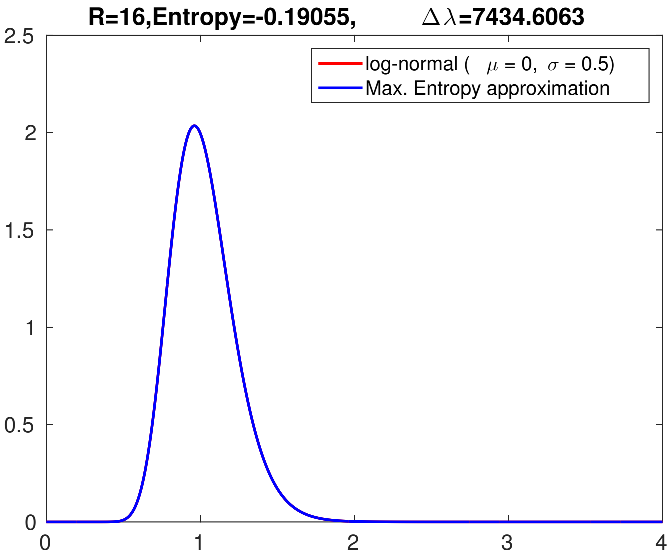

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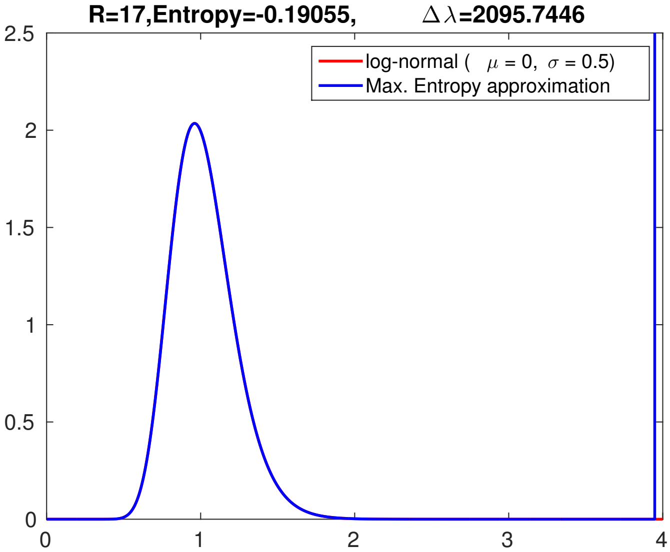

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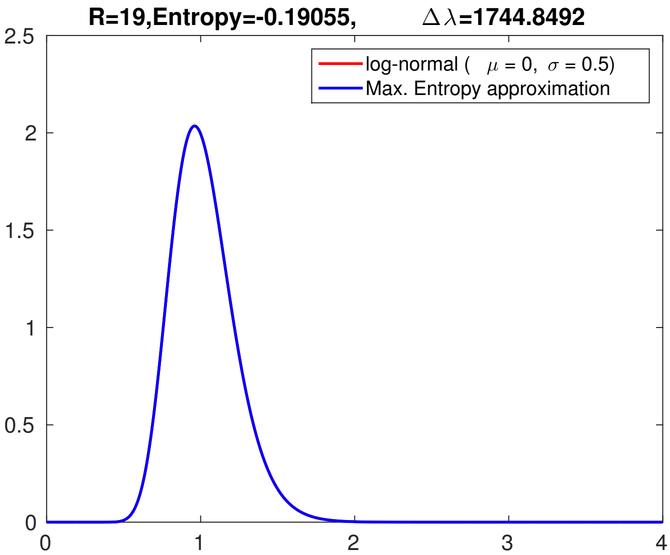

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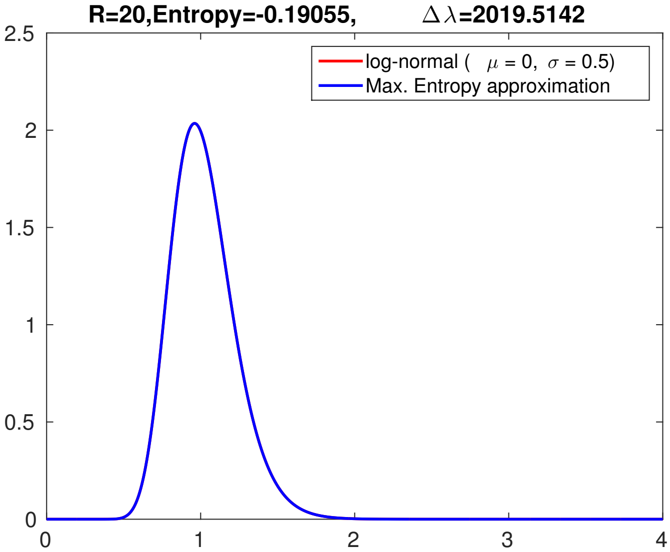

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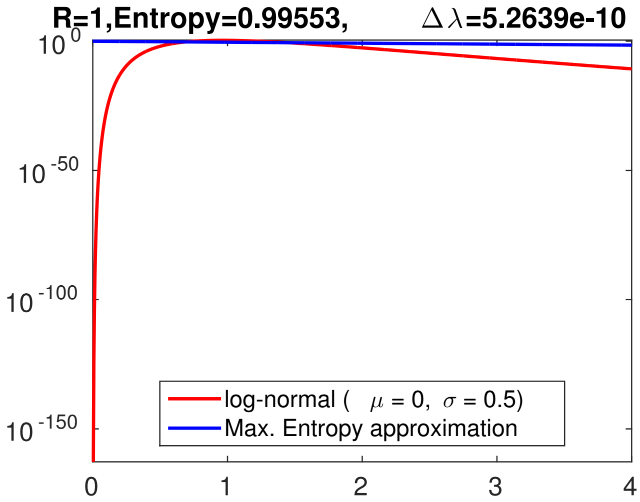
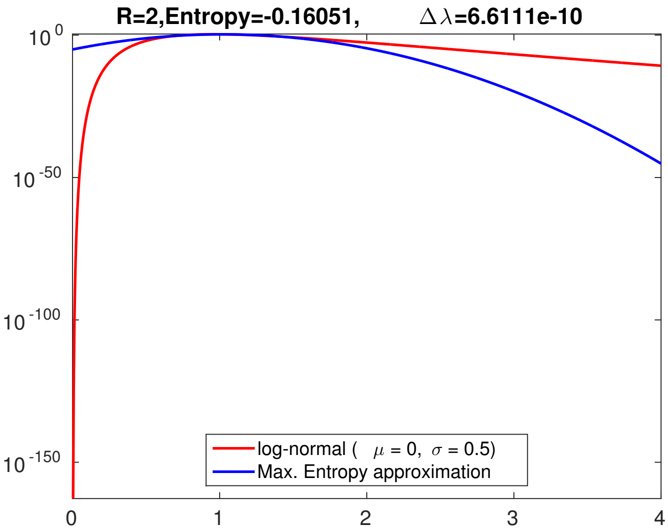


Legendre Moments ($\sigma = 0.2$, $[a, b] = [0, 4]$, semilog):

- Oscillations in the negative domain
- $\Rightarrow$ stability of the density



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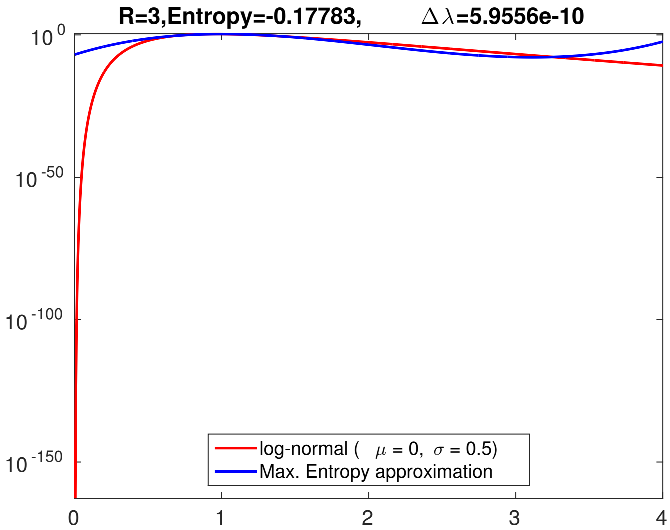

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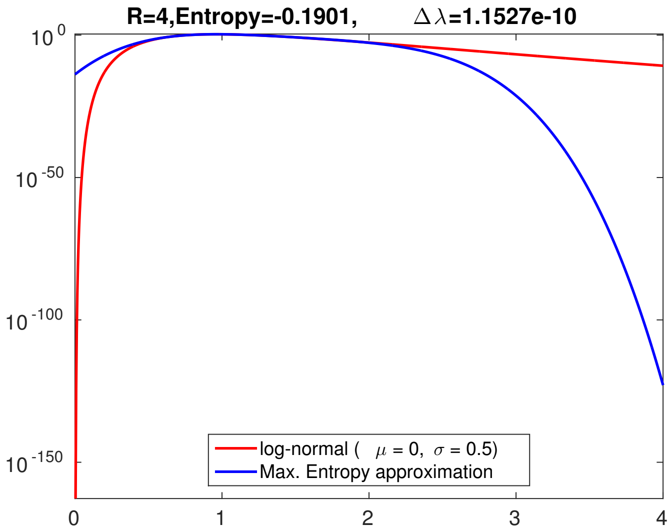

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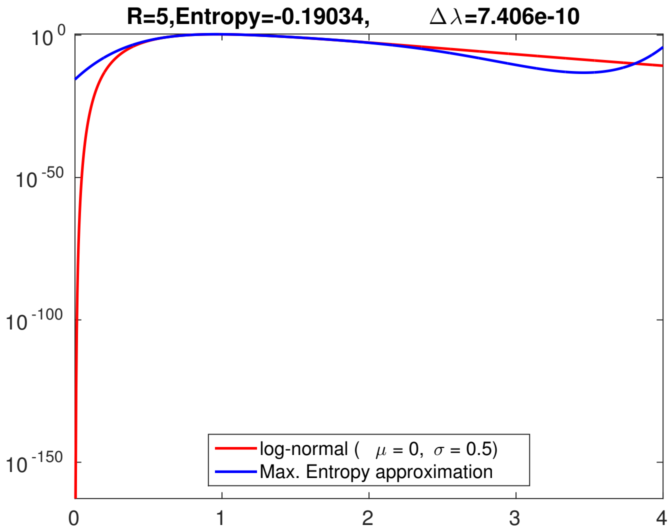

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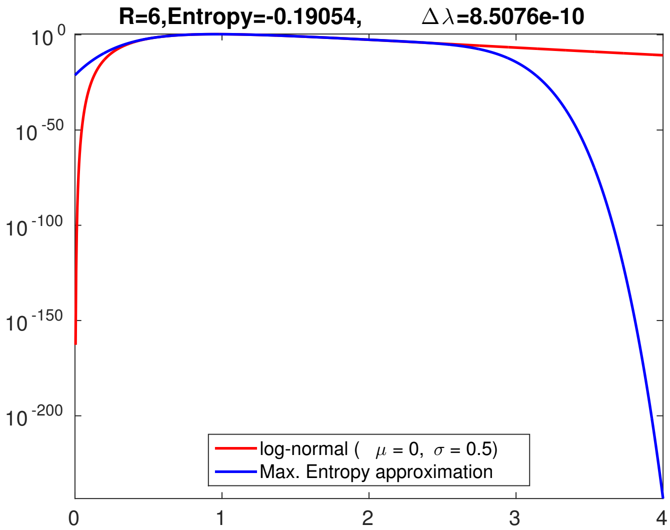

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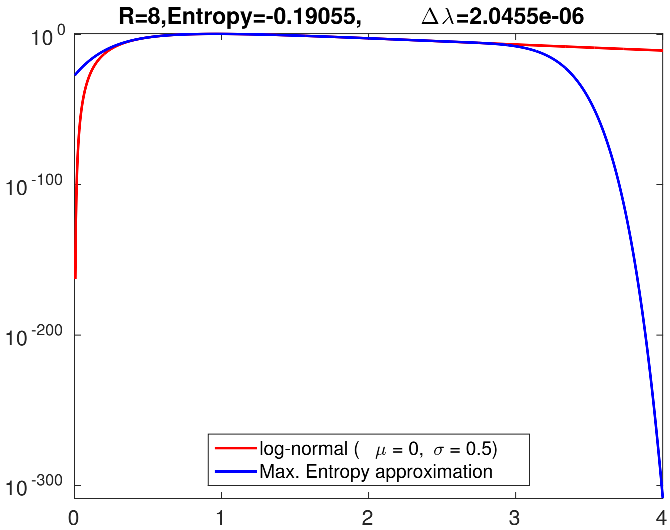

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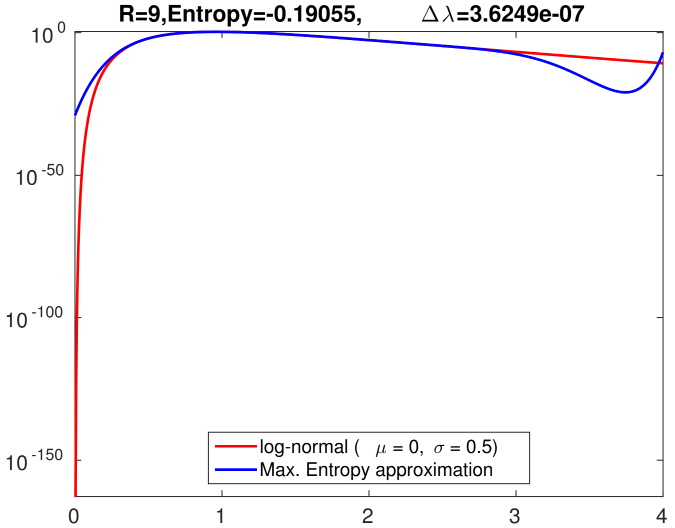

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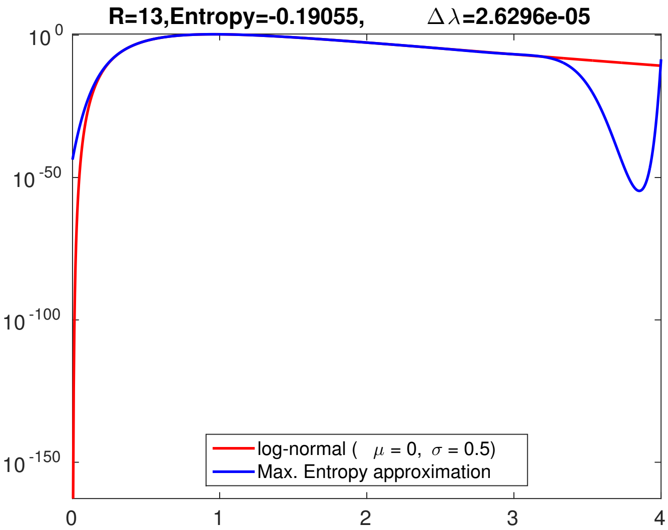

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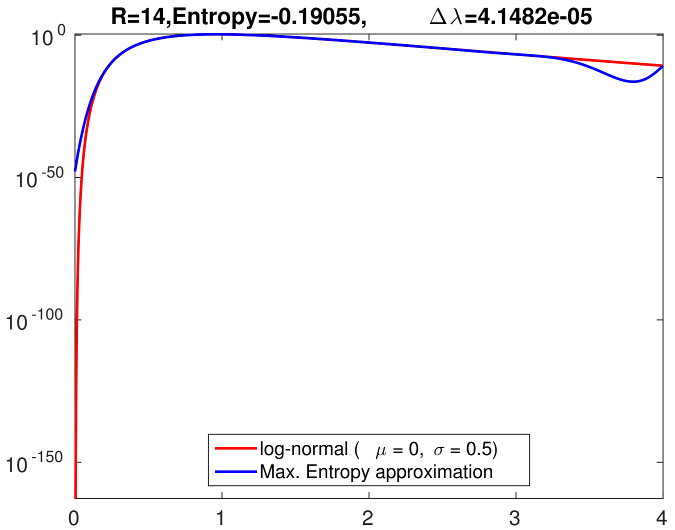

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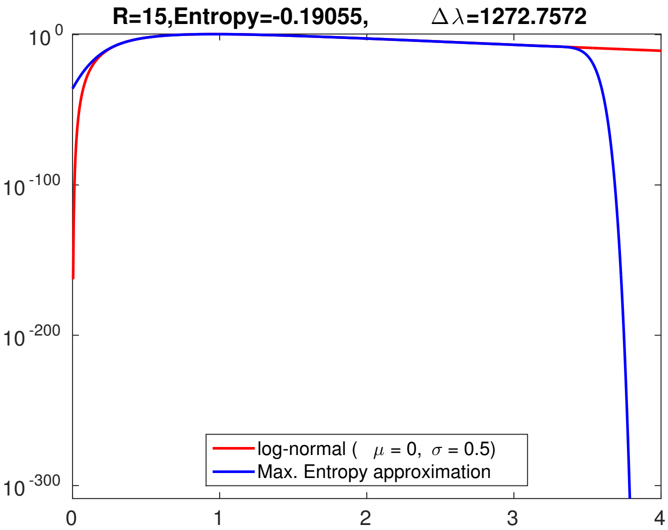

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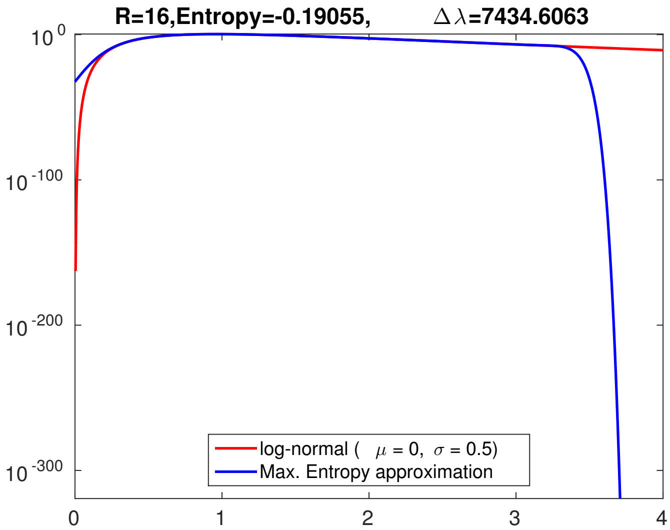

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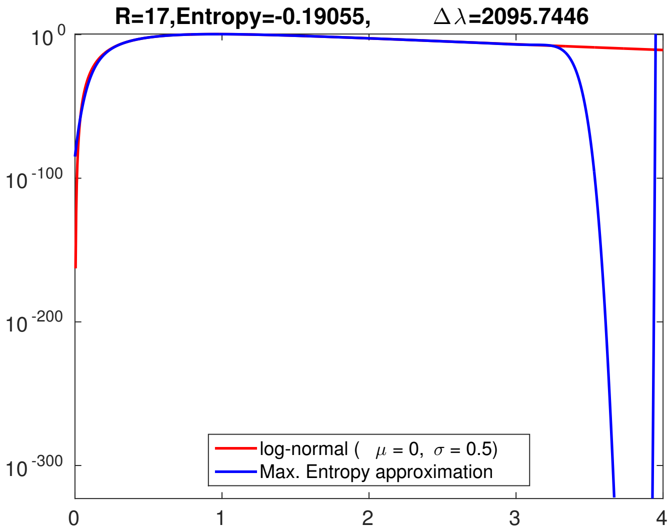

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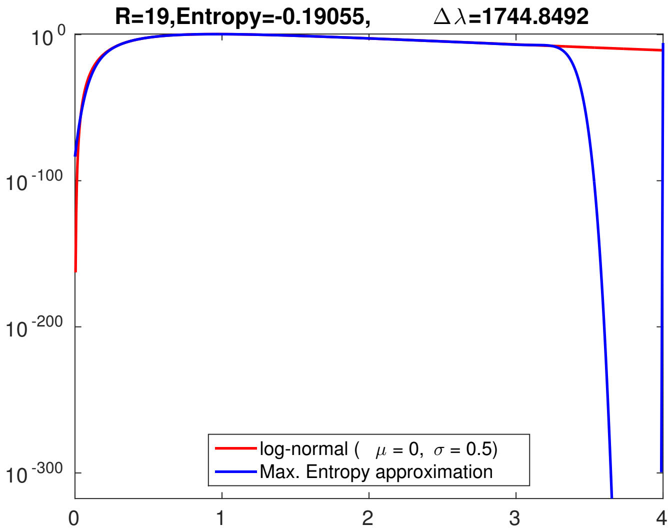

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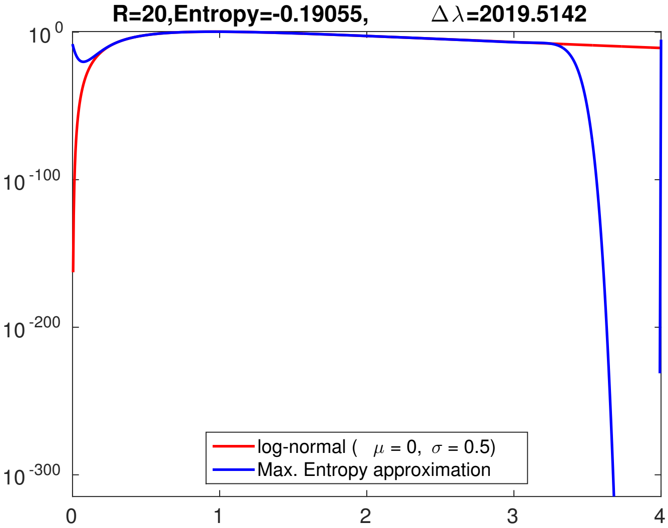

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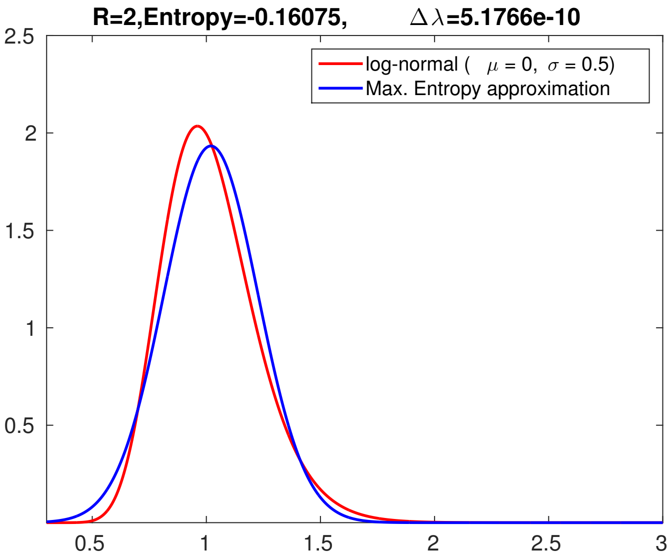
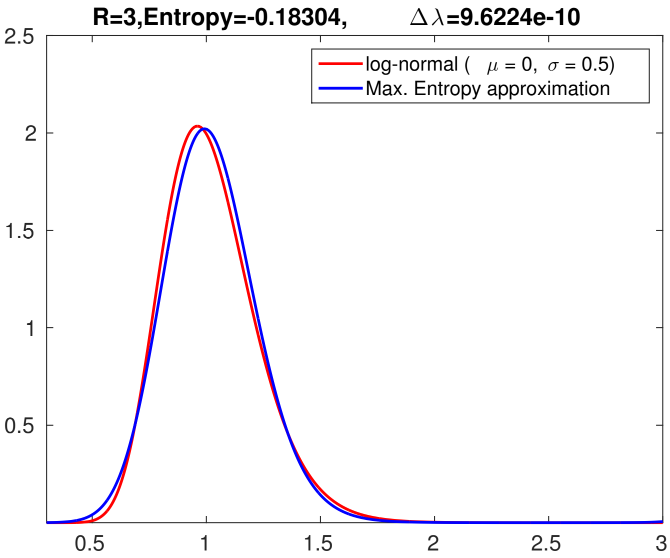


Legendre Moments ($\sigma = 0.2$, $[a, b] = [0.3, 3]$):

- Is stable and convergent for a bigger range $R \leq 14$!
- Entropy is monoton. decr. (stat. accuracy of MC is reached?)



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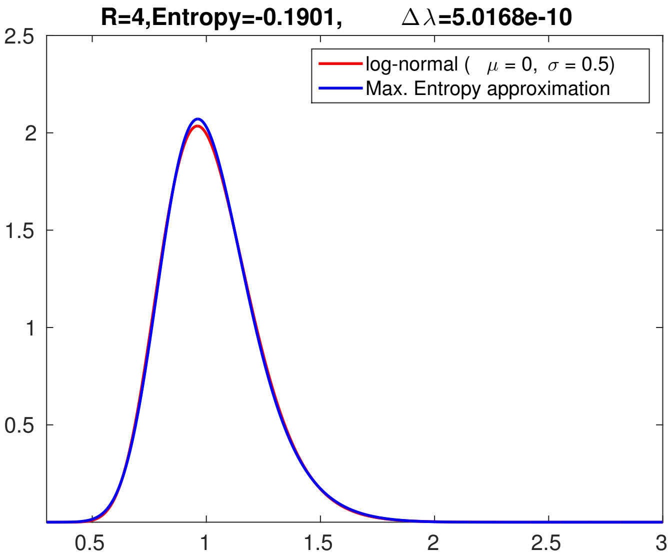

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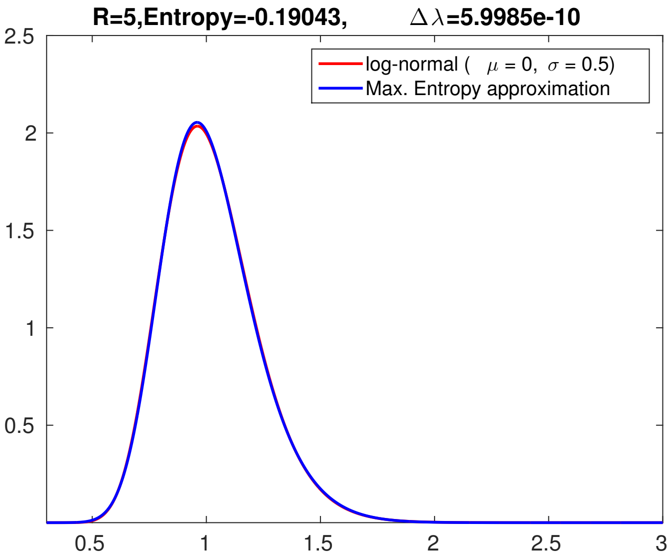

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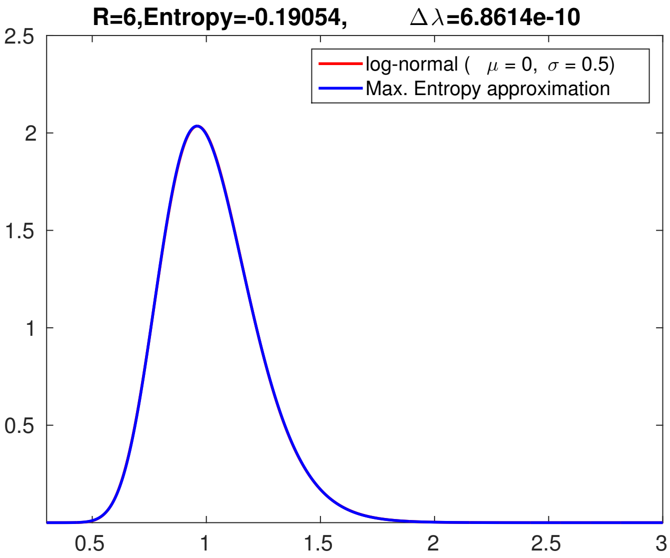

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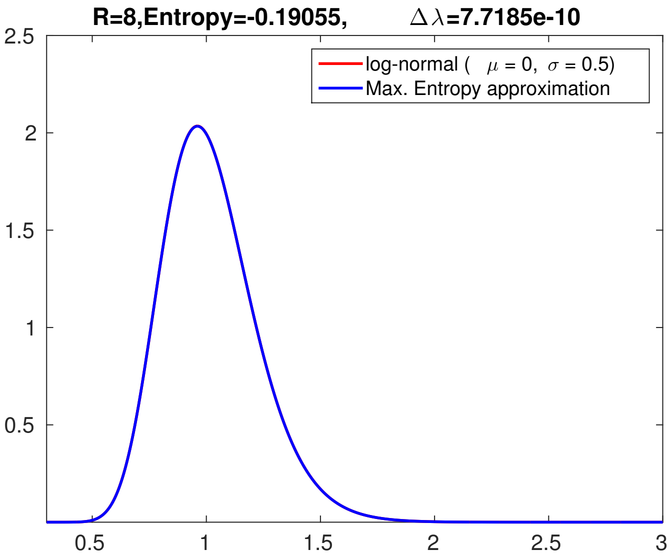

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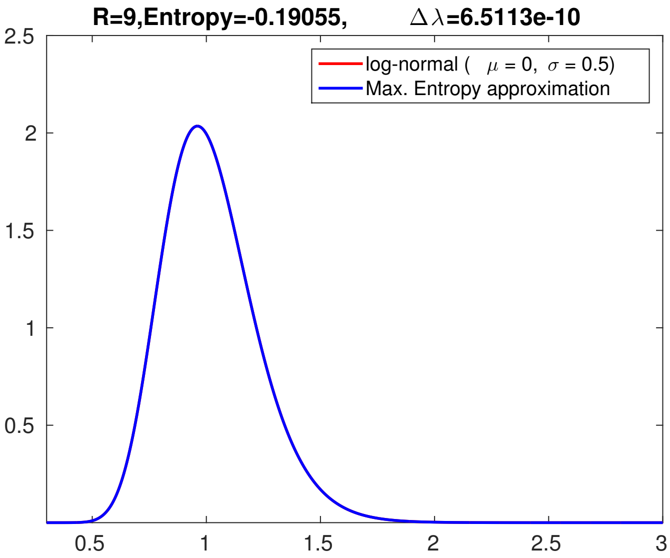

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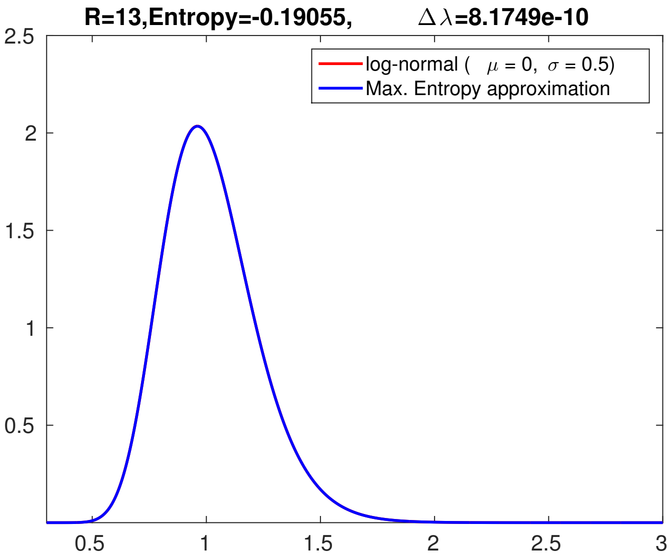

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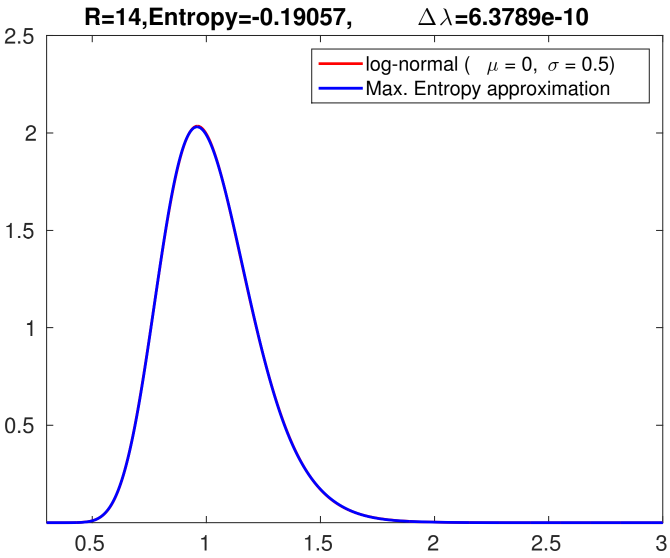

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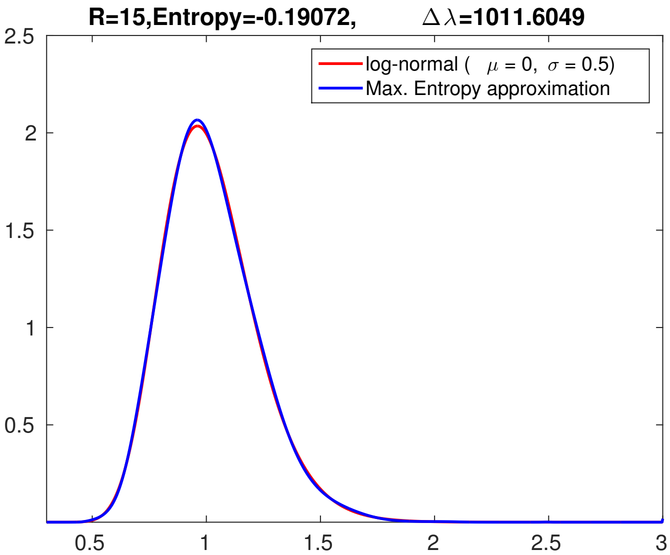

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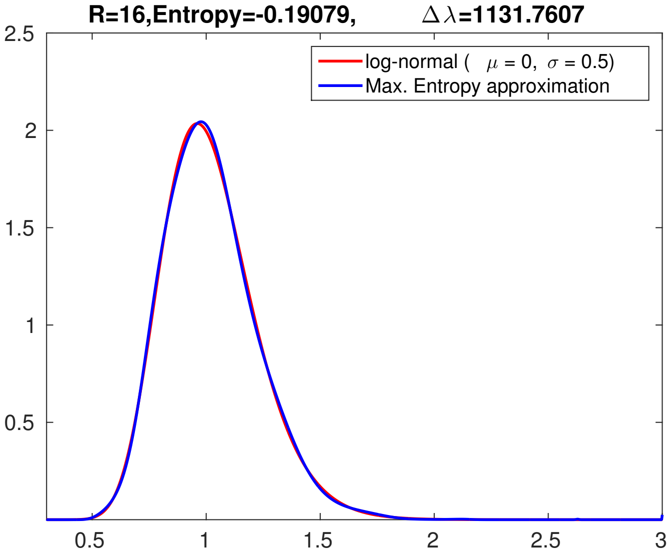

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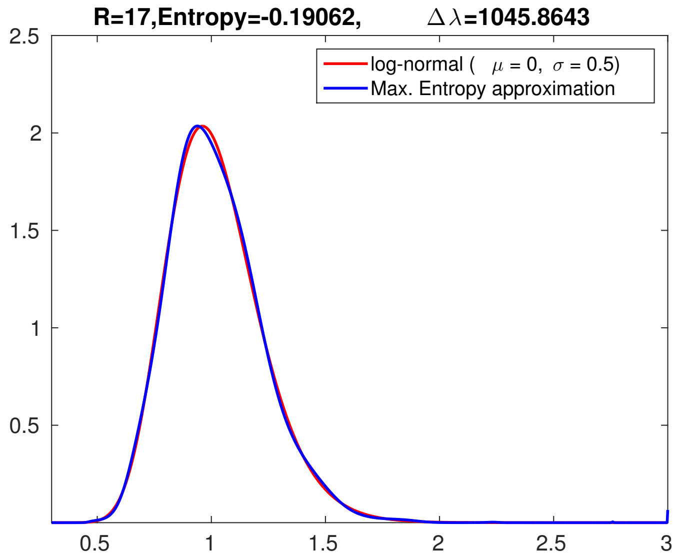

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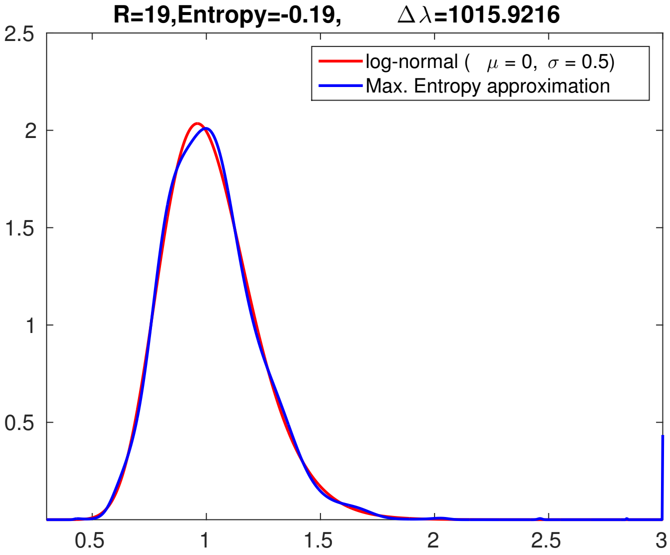

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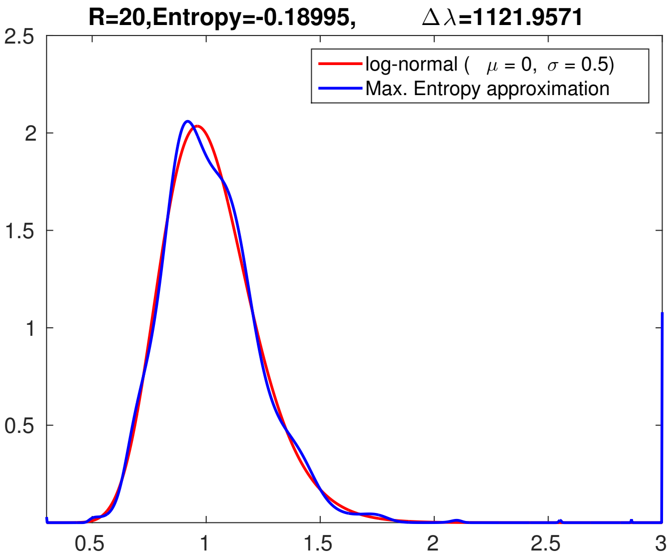

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Many open questions. . .

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