Closed-Form Information-Theoretic Roughness Measures for Mixture Densities

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Context & Motivation

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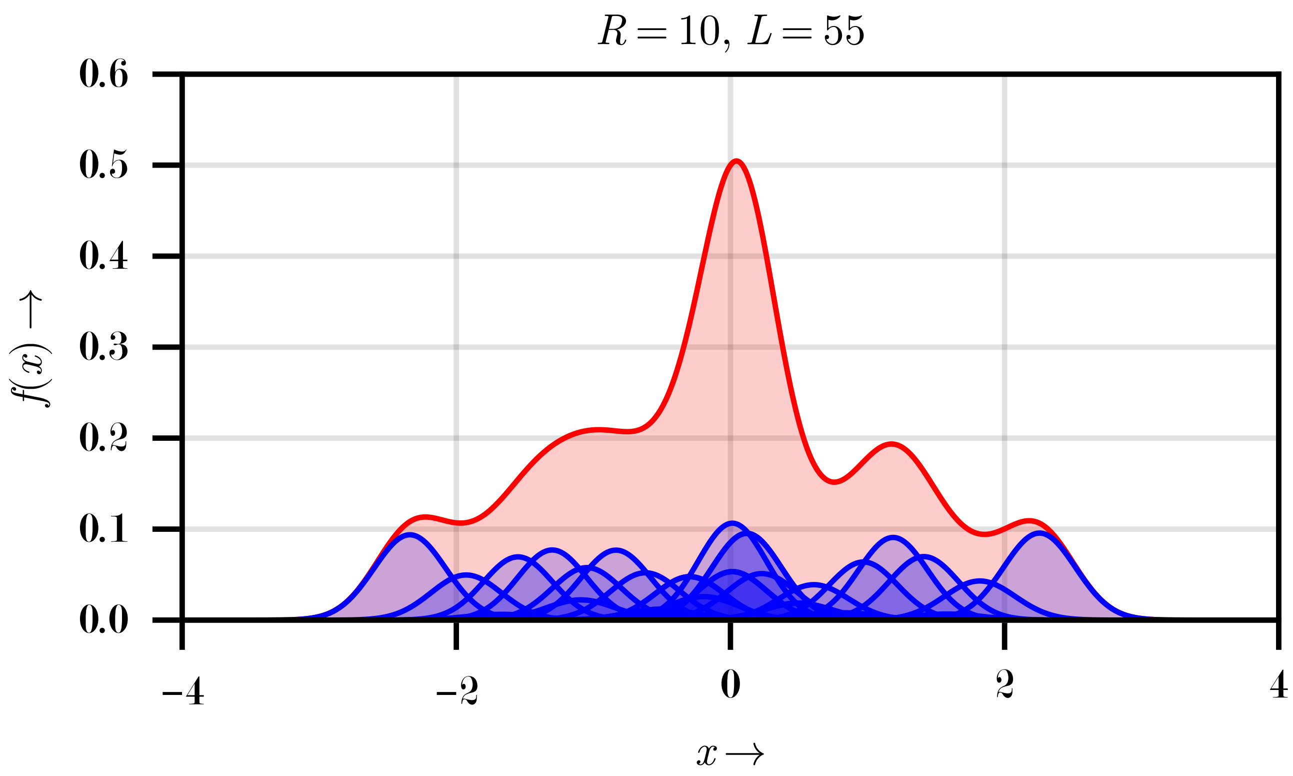
Many applications: Some specifications on probability density function given

Goal: Find cont. density that adds as little *information* as possible to specification

Example: Only single constraint $f(0) = 0.5$



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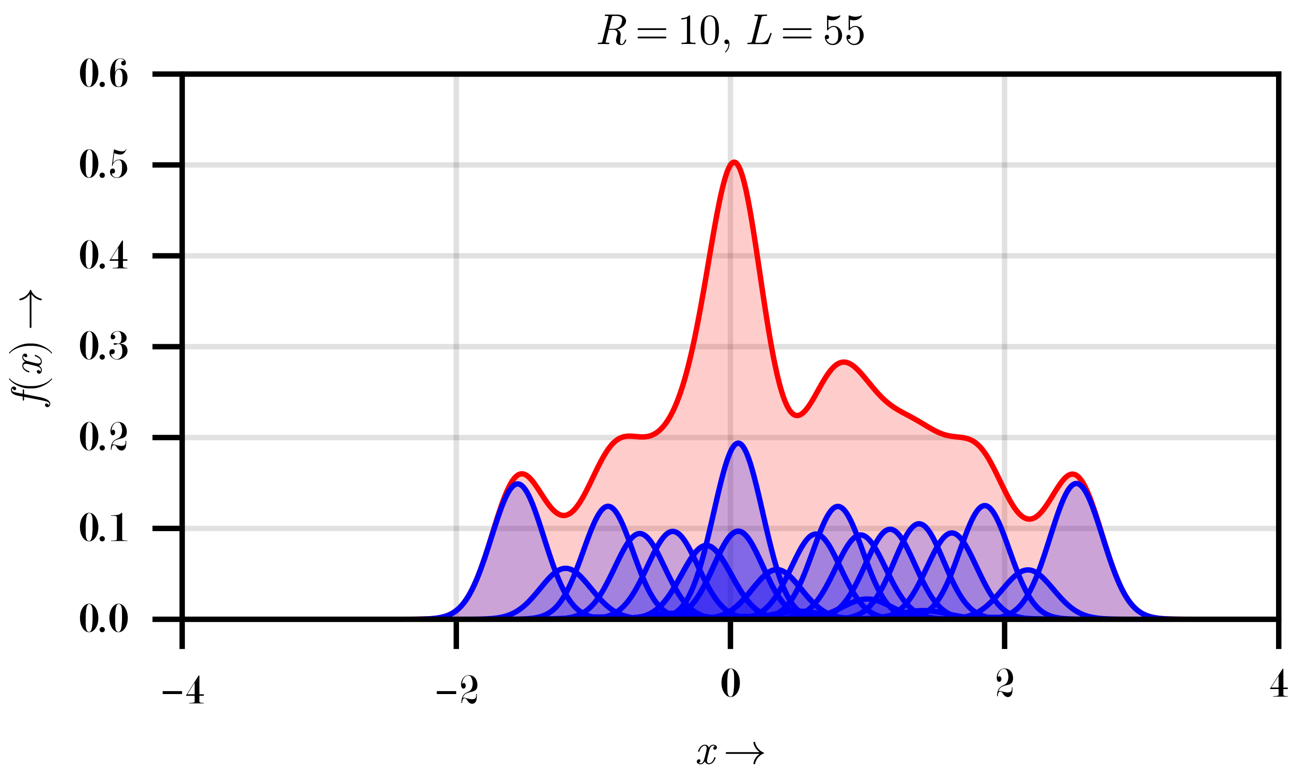

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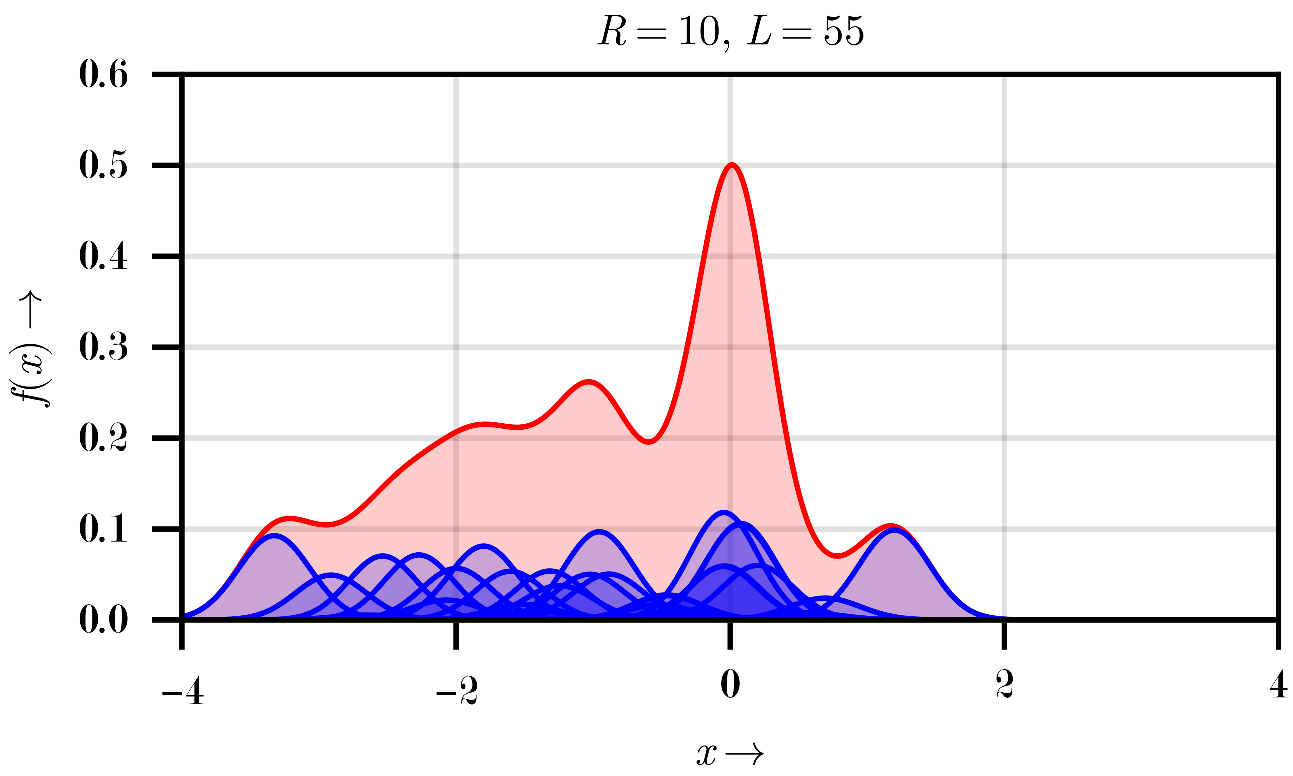

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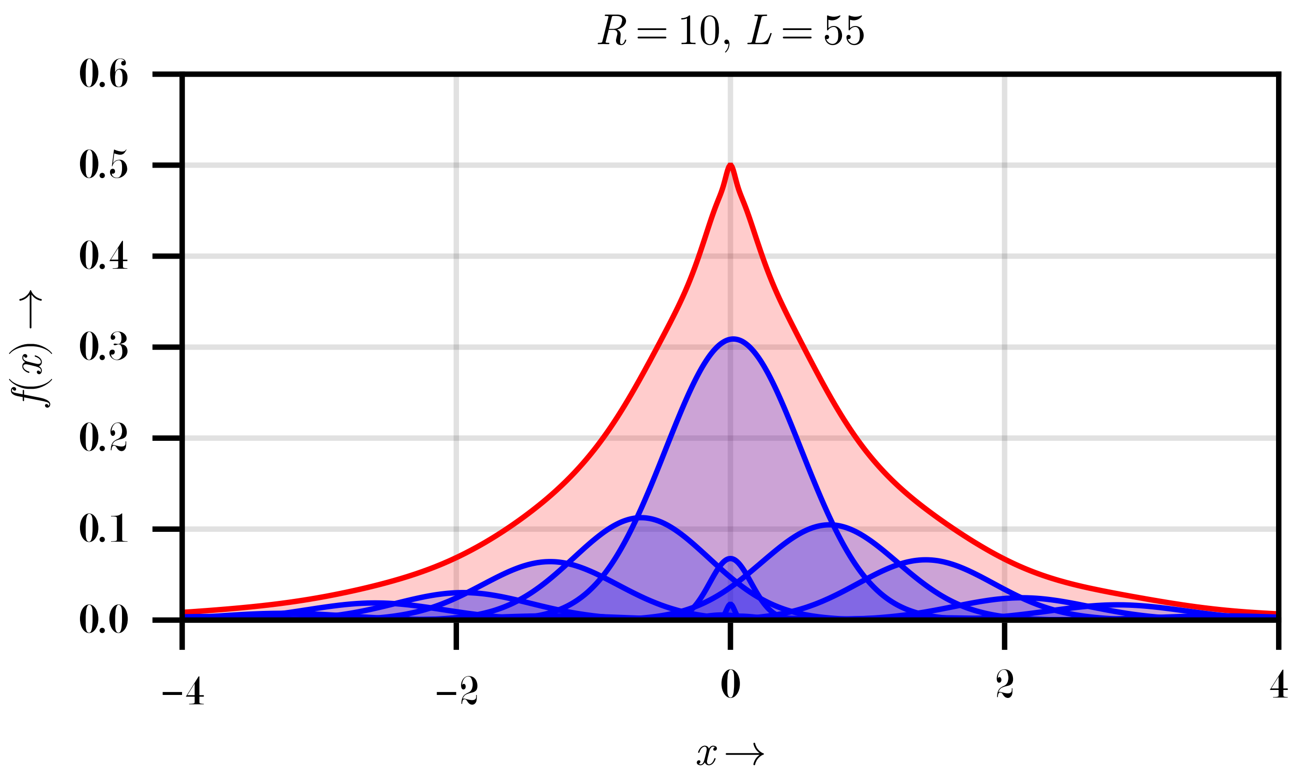

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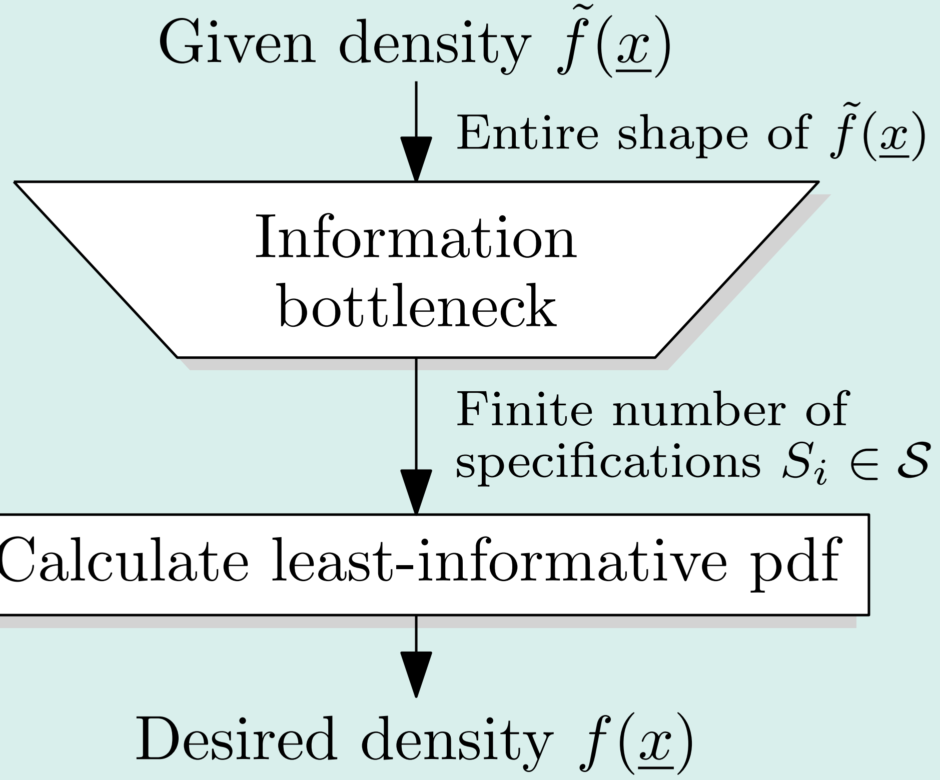
Context & Motivation

General setup:

- (Virtual) underlying true density $\tilde{f}(\underline{x})$
- Discrete set of specifications S_i



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Challenges

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Common to applications:

- Constraints do not fully characterize density
- Results in *underdetermined* optimization problem
- Some *regularizer* required

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Want to use information measure as regularizer

$\longrightarrow$ Find least-informative density under prescribed specifications

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Want to use information measure as regularizer

$\longrightarrow$ Find least-informative density under prescribed specifications

Least-informative density

- Exhibit certain smoothness
- No bumps and ripples

$\longrightarrow$ Roughness measure

Derivation of Roughness Measure

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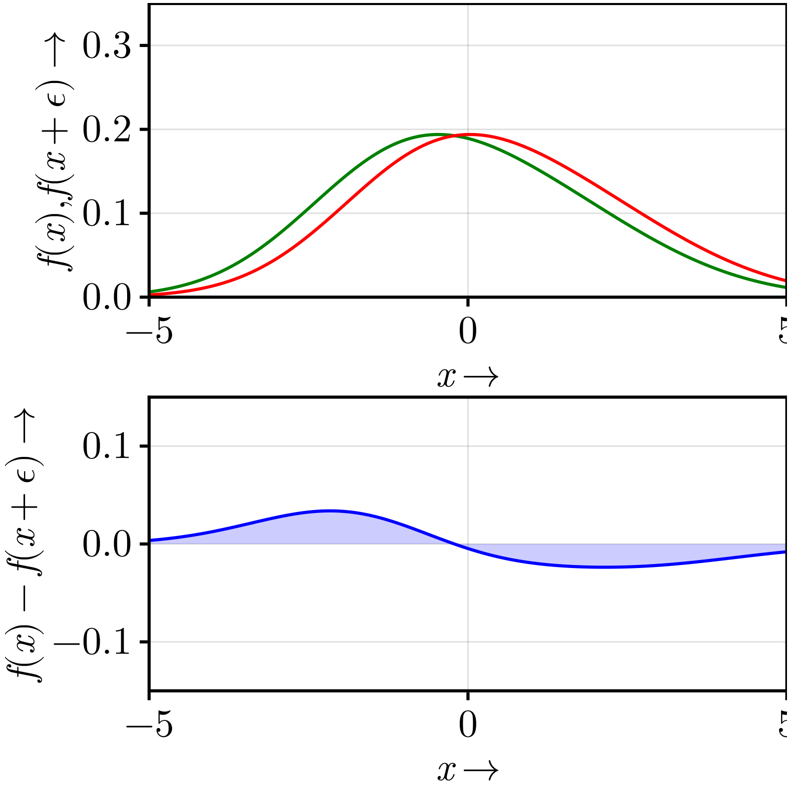
Roughness Measures - Intuition

Compare given density $f(x)$ with its shifted copy $f(x+\epsilon)$

The smoother $f(x)$: Deviation between $f(x)$ and $f(x+\epsilon)$ smaller



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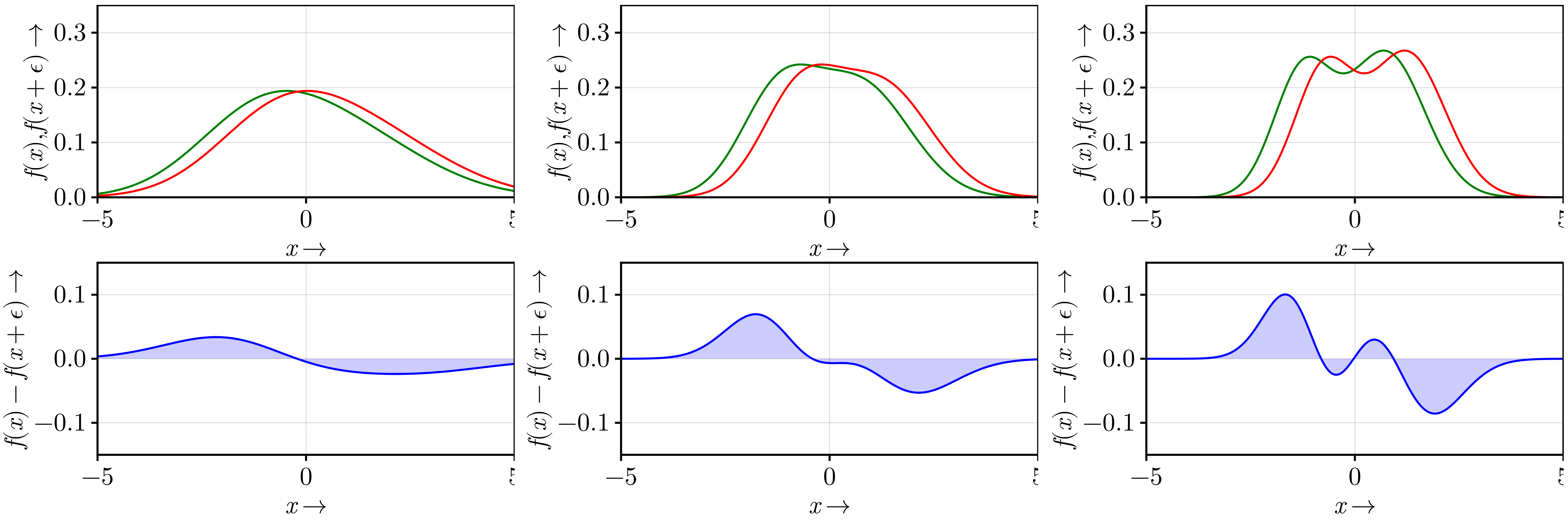

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Roughness Measures - Compare $f(x)$ and $f(x+\epsilon)$

Different measures for comparing $f(x)$ and $f(x+\epsilon)$

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Typical (**global !**) measures for comparing two densities $f(x)$ and $g(x)$

Squared integral deviation

$$D_{\mathsf{SID}}(f, g) = \int_{\mathbb{R}} \left(f(x) - g(x)\right)^2 dx$$

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Roughness Measures - Compare $f(x)$ and $f(x+\epsilon)$

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Hellinger distance

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Roughness Measures - Comparison with WSID

$$D(\epsilon) = D_{\mathsf{WSID}}\big(f(x), f(x+\epsilon)\big) = \int_{\mathbb{R}} \frac{\big(f(x) - f(x+\epsilon)\big)^2}{2\, f(x)} dx$$

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For function $h(\epsilon)\colon \mathbb{R} \to \mathbb{R}$, Taylor series expansion around ϵ_0

$$h(\epsilon) \approx h(\epsilon_0) + \frac{dh(\epsilon)}{d\epsilon} \cdot (\epsilon - \epsilon_0) + \frac{d^2 h(\epsilon)}{d\epsilon^2} \cdot (\epsilon - \epsilon_0)^2$$

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Taylor series of $D(\epsilon)$ around $\epsilon_0 = 0$ (assume regularity)

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Roughness Measures - Comparison with KL

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$$= \underbrace{\int_{\mathbb{R}} f'(x)\, dx}_{0} \cdot \epsilon + \int_{\mathbb{R}} \Bigg\{ \frac{\big[f'(x)\big]^2}{f(x)} \underbrace{- f''(x) \Bigg\}}_{0} dx \cdot \epsilon^2$$

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2nd Derivation Based on Fisher Information

Review: Fisher Information with Respect to Parameter

For **location parameter** θ, the likelihood is given by $f(x|\theta) = f(x+\theta)$, the score is

$$s(x|\theta) = \frac{\partial}{\partial\theta} \log\big(f(x+\theta)\big) = \frac{\partial f(x+\theta)}{\partial\theta} \frac{1}{f(x+\theta)} = \frac{\partial f(x+\theta)}{\partial x} \frac{1}{f(x+\theta)}$$

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The Fisher information can be rewritten as

$$I_F(\theta) = \int_{\mathbb{R}} \left[\frac{\partial f(x+\theta)}{\partial x} \frac{1}{f(x+\theta)}\right]^2 f(x+\theta) dx = \int_{\mathbb{R}} \left[\frac{\partial f(x+\theta)}{\partial x}\right]^2 \frac{1}{f(x+\theta)} dx$$

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As $I_F(\theta)$ does not depend on θ anymore, we have

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That looks familiar!

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Result and Generalization to Multivariate Case

All derivations give **Fisher Information Number (FIN)**

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Generalization to D dimensions

$$I_F^{\mathcal{M}}(f) = \int_{\{\mathbb{R}^D,\, f>0\}} \frac{\left|\nabla f(\underline{x})\right|^2}{f(\underline{x})} \, d\underline{x}$$

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Root Mixtures

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Root Mixtures

Define square root mixtures as

$$r(\underline{x}) = \sum_{i=1}^{R} v_i \, r_i(\underline{x}) \qquad v_i \text{ arbitrary for now}$$

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Conversion of square root mixture to mixture in original mixture space

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Expression contains redundant terms as $r_i(\underline{x}) \, r_j(\underline{x}) = r_j(\underline{x}) \, r_i(\underline{x})$ for $i \neq j$

Fisher Information Number - Challenges & Key Idea

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Fisher Information Number - Challenges & Key Idea

Define two density spaces:

- Original space of mixture densities $\mathcal{M}$
- Space of root mixture densities $\mathcal{R}$

Root Mixture Space	Original Mixture Space
$\mathcal{R}$	$\mathcal{M}$
$r(\underline{x})$	$f(\underline{x})$

$$r^2(\underline{x}) = f(\underline{x}) \quad \longrightarrow$$

$$\longleftarrow \quad r(\underline{x}) = \sqrt{f(\underline{x})}$$

$$4 \int_{\underline{x} \in \mathbb{R}^D} \left| \nabla r(\underline{x}) \right|^2 d\underline{x} = I_F^{\mathcal{R}}(r) = I_F^{\mathcal{M}}(f) = \int_{\{\mathbb{R}^D,\, f>0\}} \frac{\left| \nabla f(\underline{x}) \right|^2}{f(\underline{x})} \, d\underline{x}$$

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Optimization

Optimization

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Given:

- Set of specifications $S_i(f) = 0\,,\ S_i \in \mathcal{S}$ on $f(\underline{x})$
- Basic constraints on $f(\underline{x})$, i.e., unit integral constraint

Desired:

- Find parameters of least-informative root mixture under constraints

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Optimization problem:

$$\begin{aligned} \min_{r \in \mathcal{R}} \quad & I_F^{\mathcal{R}}(r) \\ \text{s.t.} \quad & f = r^2 \\ & S_i(f) = 0\,,\ S_i \in \mathcal{S} \end{aligned}$$

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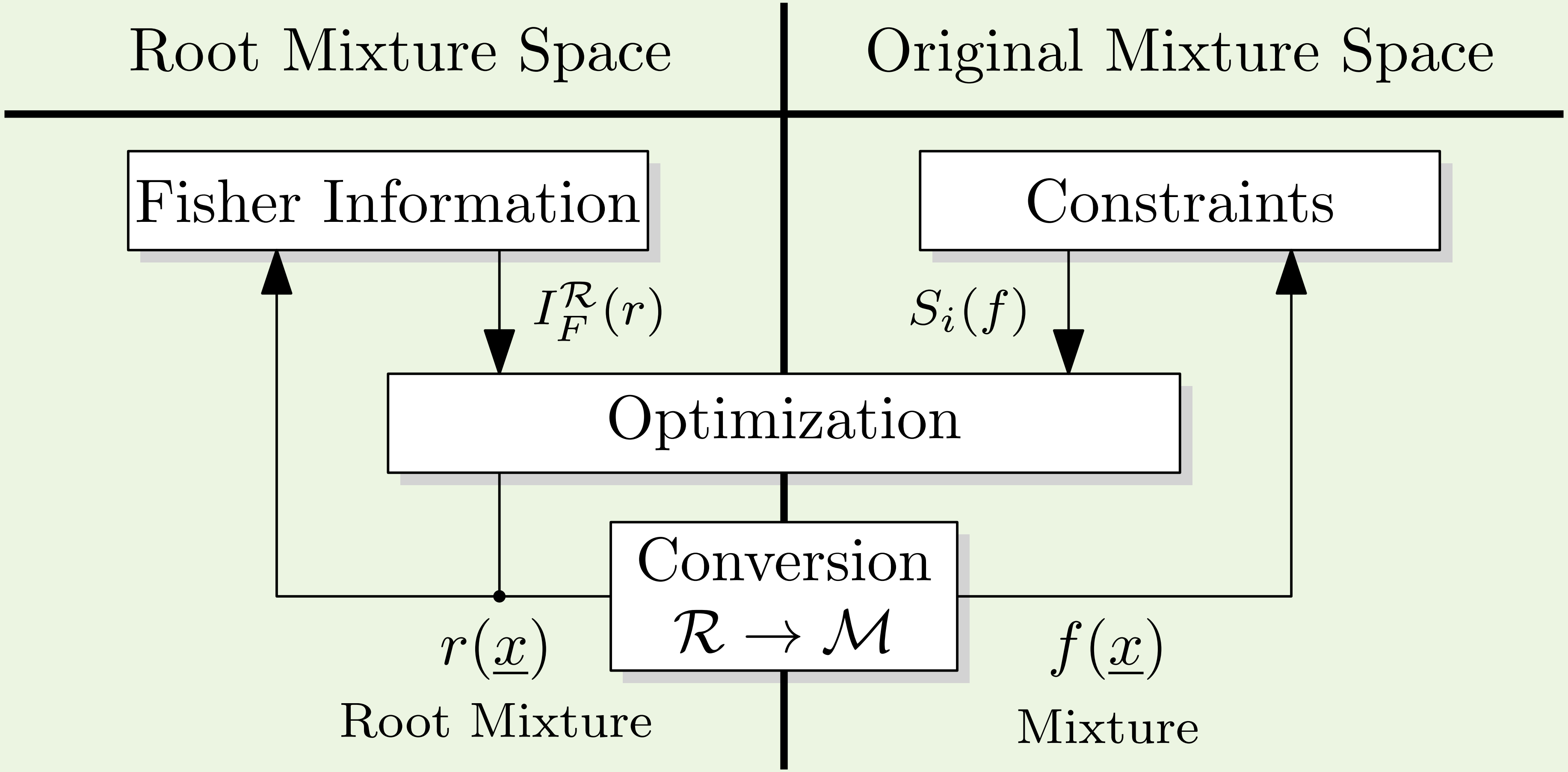
Optimization

Tandem processing in root mixture space space $\mathcal{R}$ and original mixture space $\mathcal{M}$



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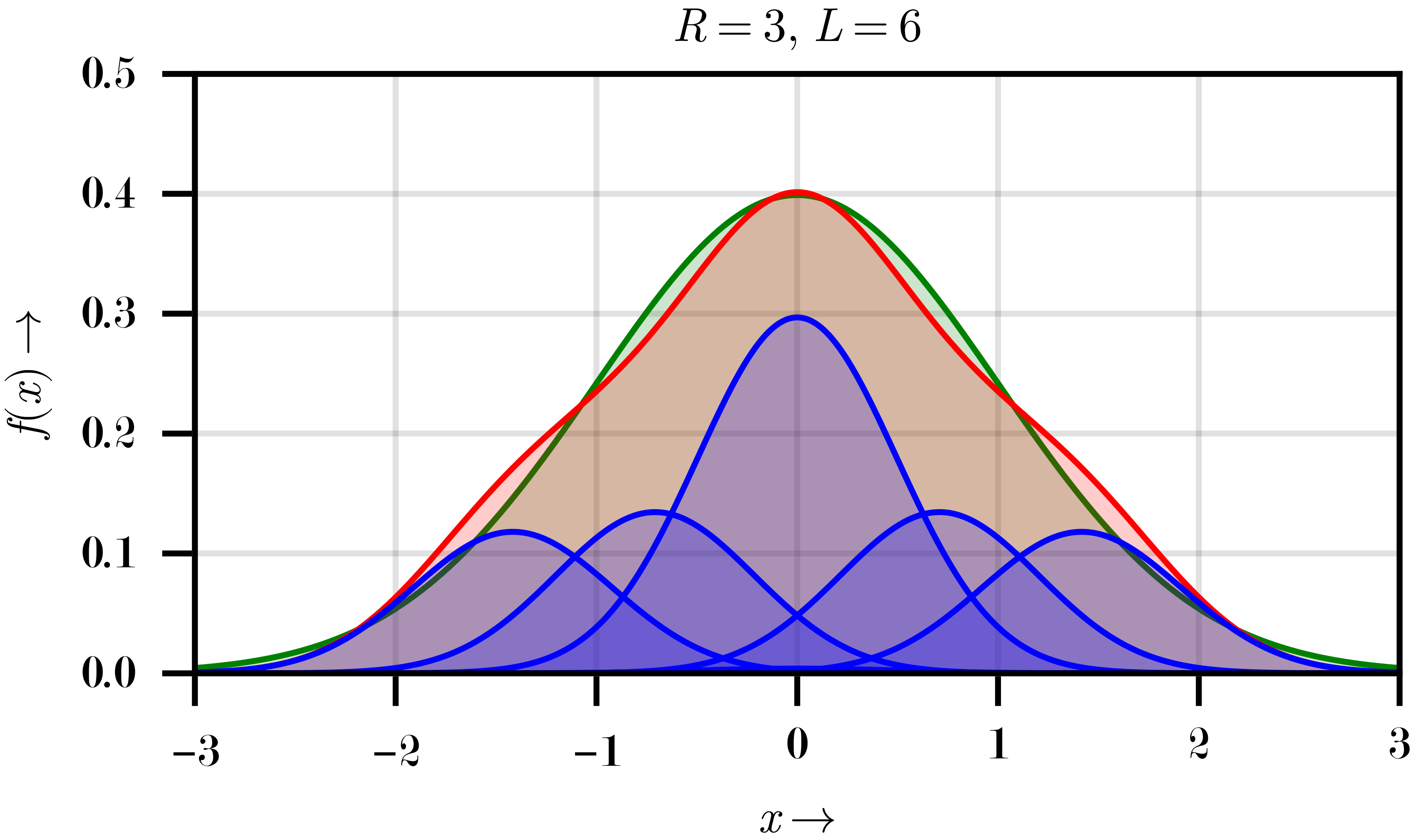
Examples

Example - Gaussian Mixture with zero mean, unit variance

$R \in \{3, 4, 5\}$ root mixture components, $L = R \cdot (R+1)/2 \in \{6, 10, 15\}$ mixture components



avoid trivial solution by bounding variance of components

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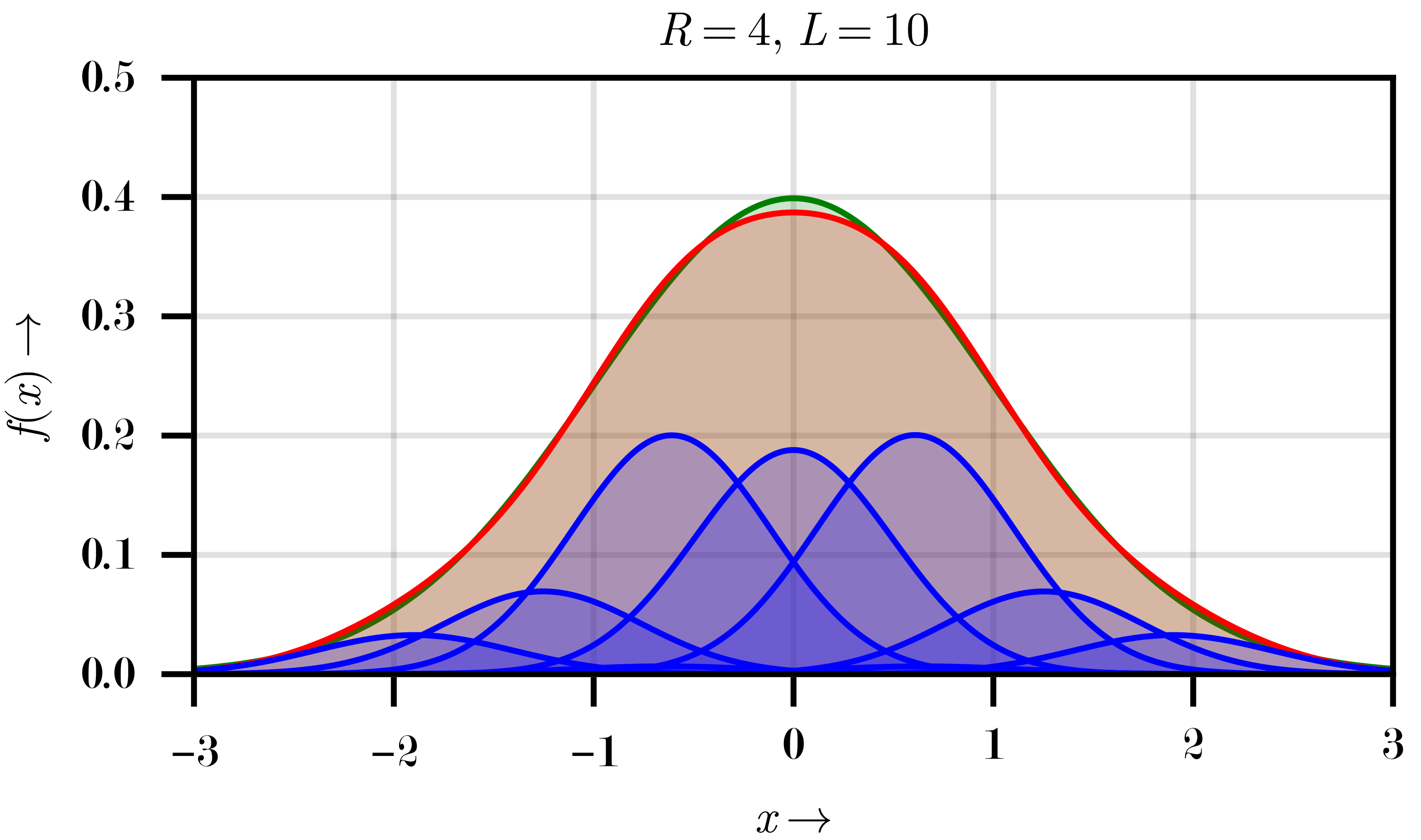

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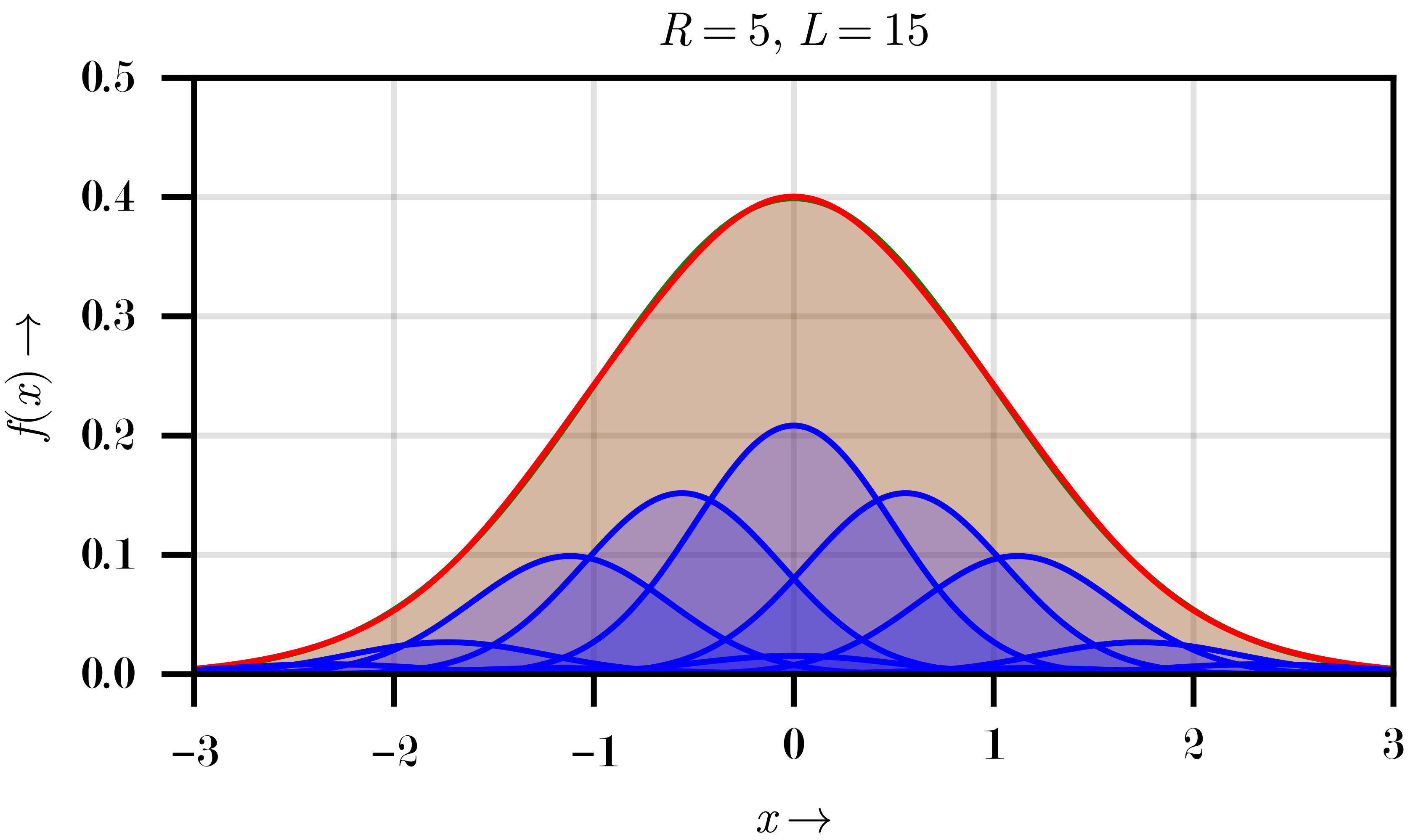

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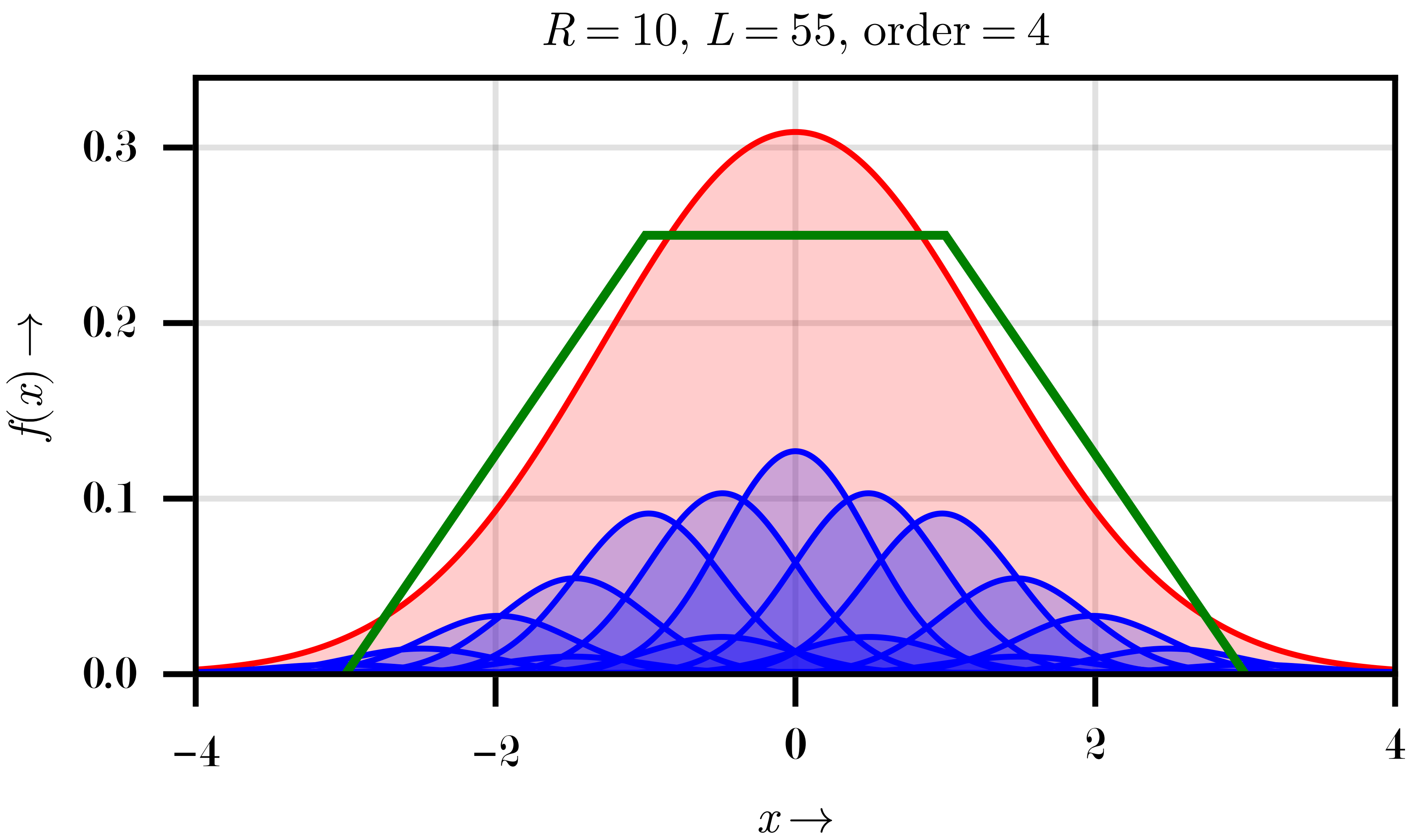
Example - Gaussian Mixture with Higher-Order Moments

$R = 10$ root mixture components, $L = R \cdot (R+1)/2 = 55$ mixture components



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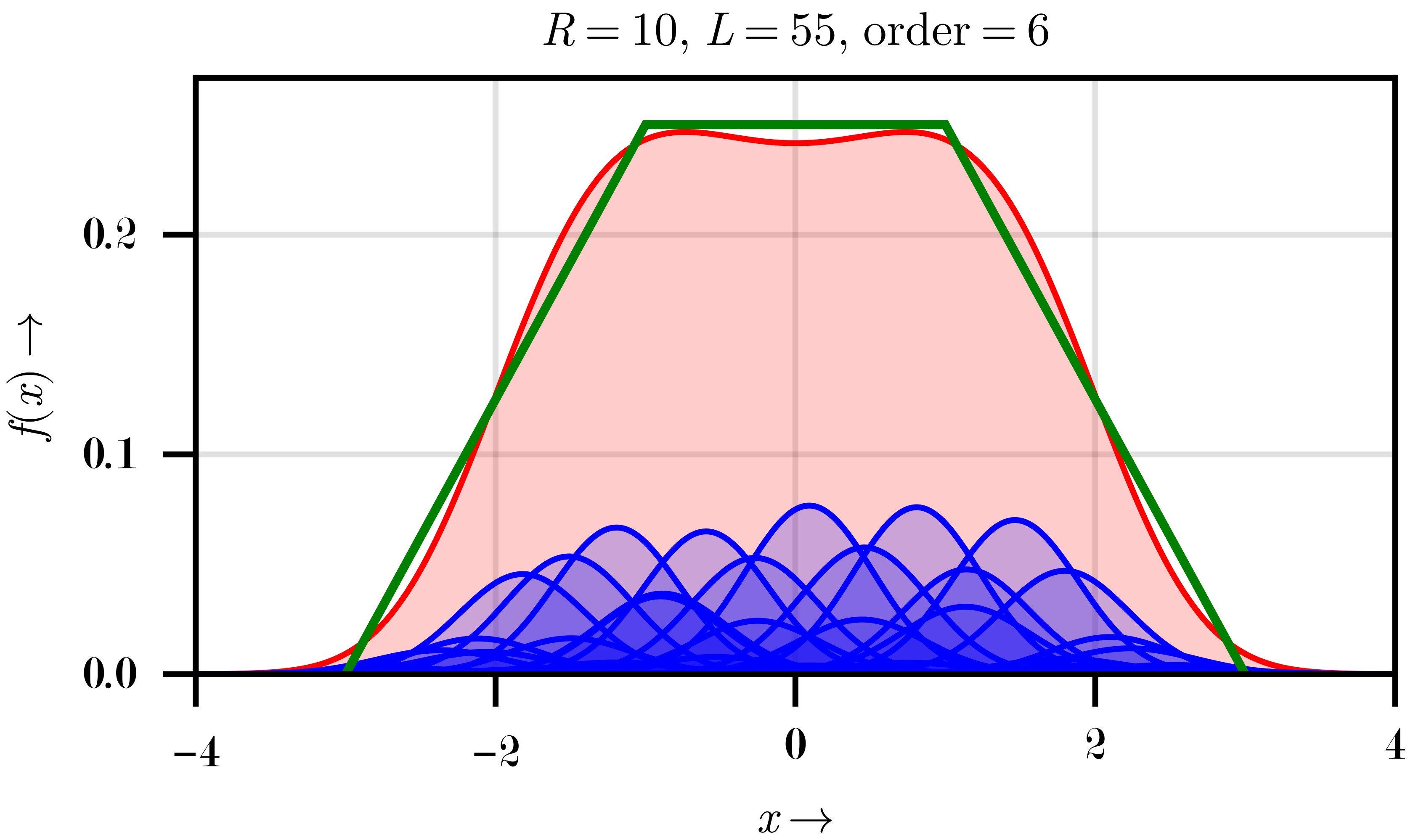

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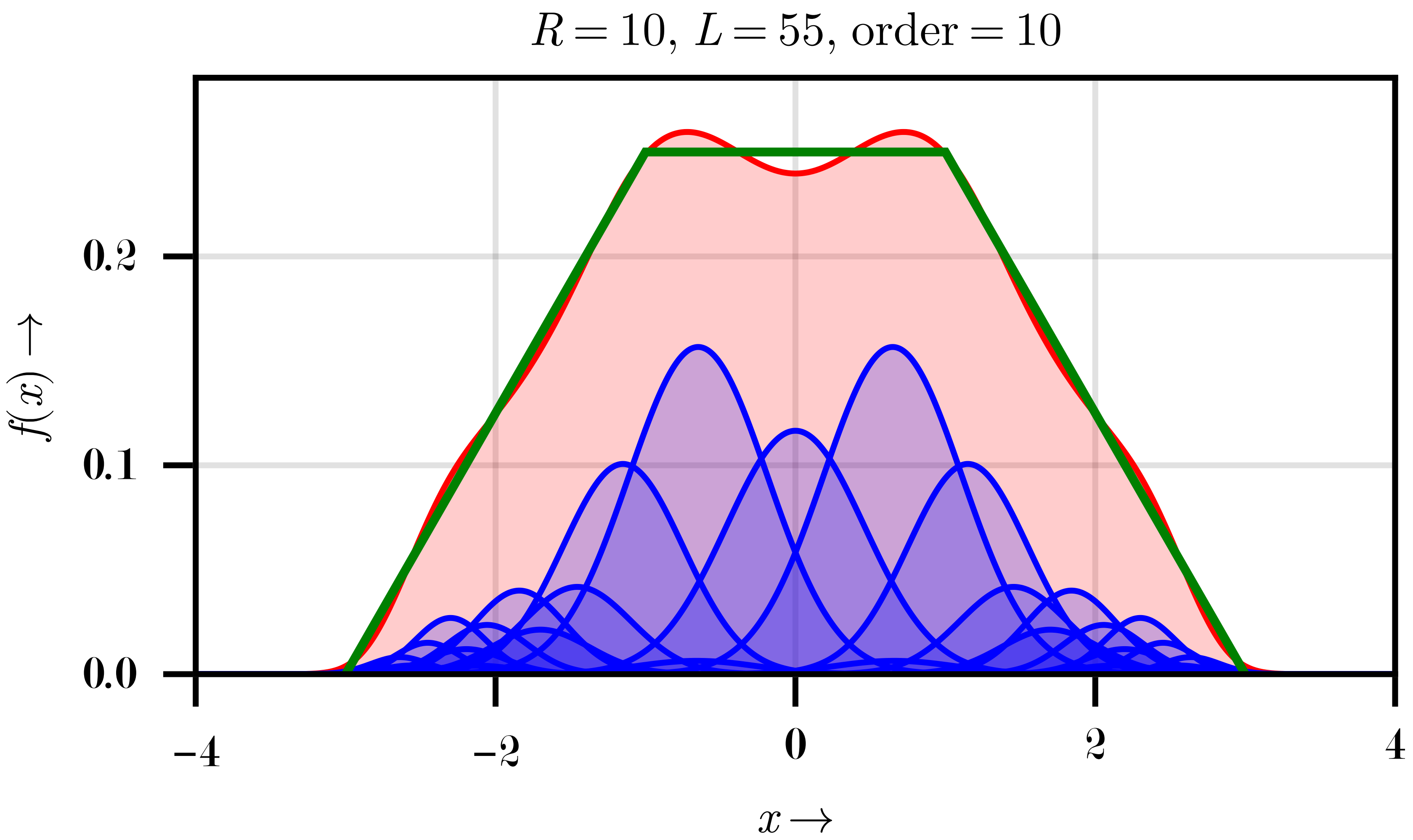
Example - Gaussian Mixture with Higher-Order Moments

$R = 10$ root mixture components, $L = R \cdot (R+1)/2 = 55$ mixture components



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Conclusion & Outlook

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Conclusions

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Closed-form solution for root mixtures

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Closed-form solution for root mixtures

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Versatile tool for optimal reconstruction
of continuous densities
from sparse specifications