Add Isotropic Gaussian Kernels at Own Risk

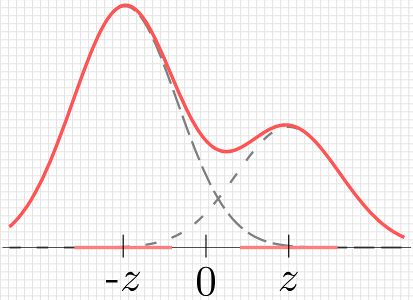
More and More Resilient Modes in Higher Dimensions

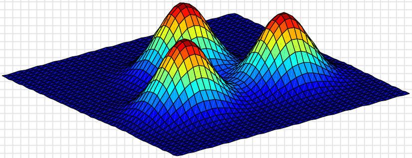
Herbert Edelsbrunner, BRITTANY TERESE FASY, and Günter Rote

Symposium on Computational Geometry 2012
Chapel Hill, North Carolina

18 June 2012

Counting Modes and Critical Points





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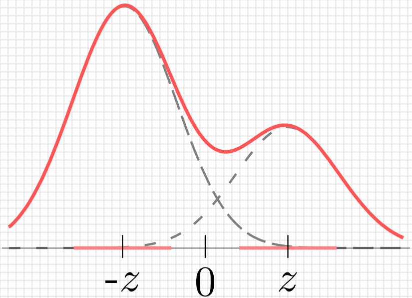

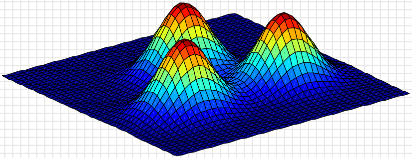

Definition

A *critical point* is a point with a zero gradient.

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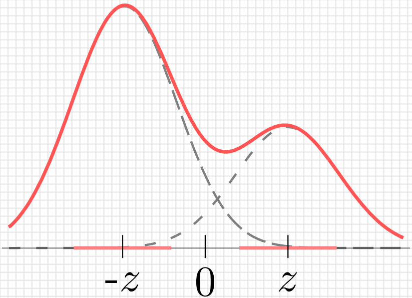

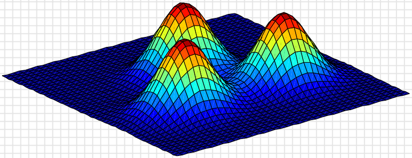

Definition

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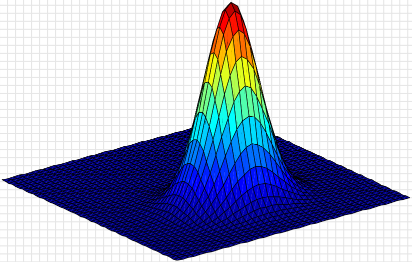
Definition

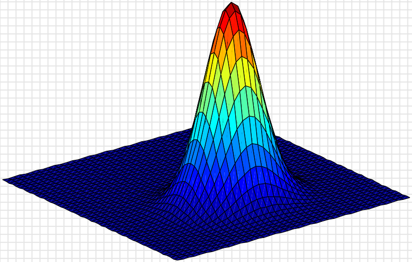
A *mode* is a local maximum.

How Many Modes (Local Maxima)?



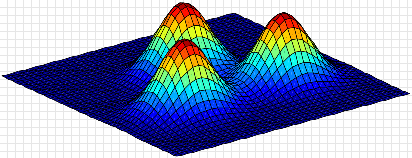
How Many Modes (Local Maxima)?

In the begining, we see 1 local maximum.



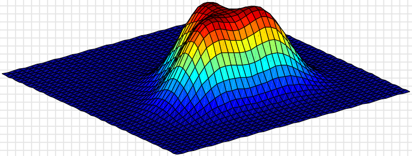
How Many Modes (Local Maxima)?

At the end, we see 3 local maxima.



How Many Modes (Local Maxima)?

In the middle, we see 4 local maxima.



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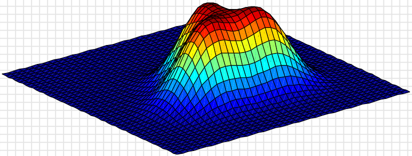

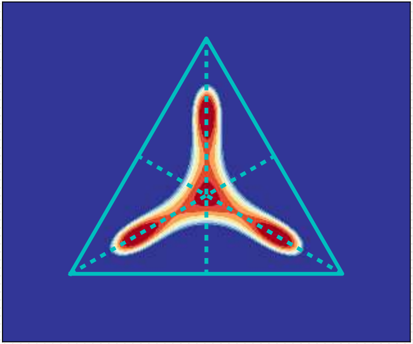

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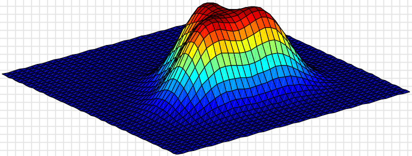

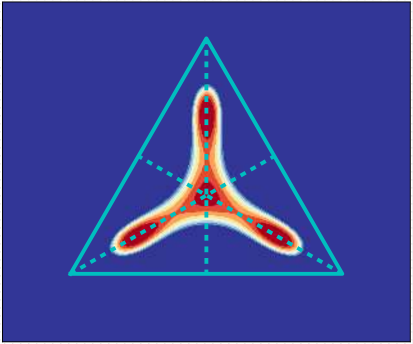

Existence proven in [M. Carreira-Perpiñán and C. Williams, Scotland 2003].

Brief Overview

- Define Gaussian kernel and mixture.

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- Analyze 1-dimensional mixtures.

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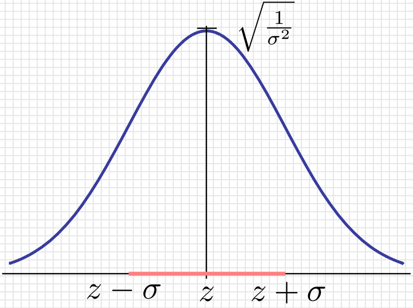
- Define Gaussian kernel and mixture.
- Analyze 1-dimensional mixtures.
- Locate and count all critical points of an n-dimensional mixture.
- Locate and count all modes of an n-dimensional mixtures.
- (Describe the resilience of the ghost mode.)

Gaussian Kernel

Definition

$$g_z(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-z)^2}{2\sigma^2}}$$



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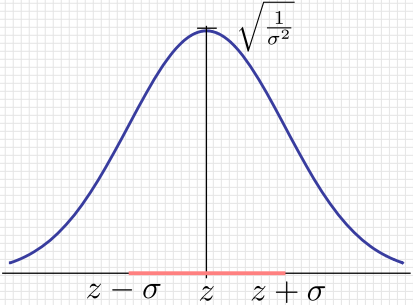

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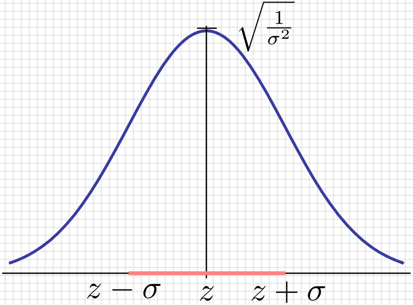

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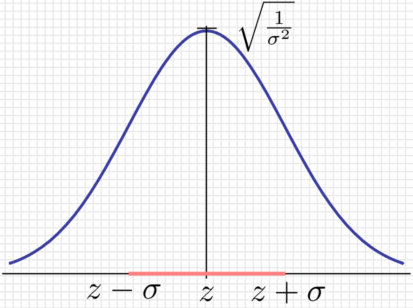

Standardized Gaussian Kernel

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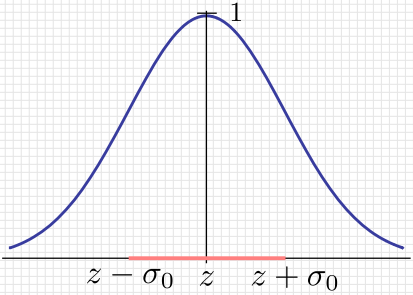
$$g_z(x) = e^{-\pi(x-z)^2}$$



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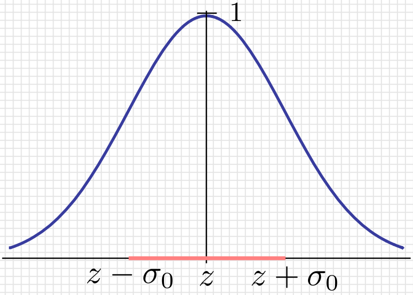

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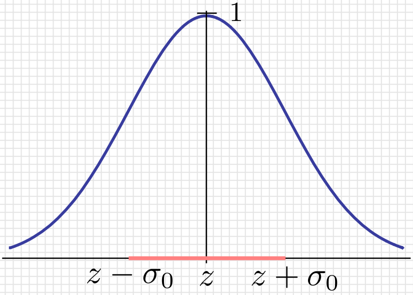

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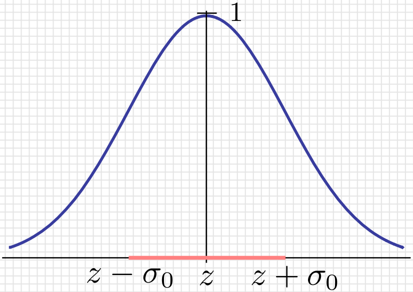

n-Dimensional Isotropic Gaussian Kernel

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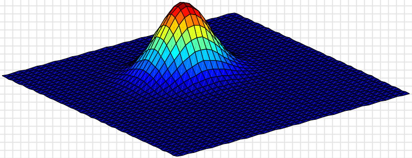

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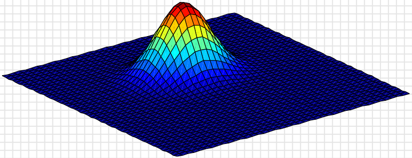

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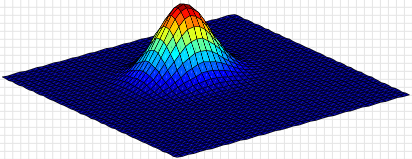

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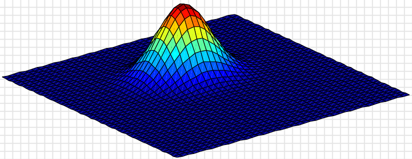
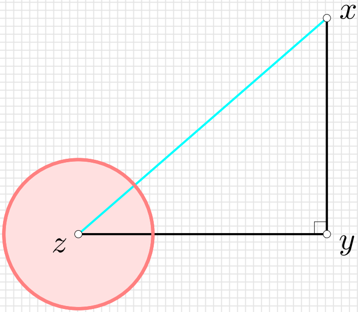


Separability of the Gaussian Kernel

Separability Lemma

$e^{-\pi||x-z||^2}$



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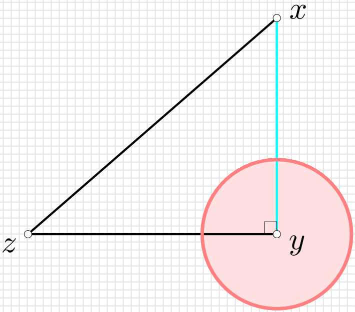
$$e^{-\pi||x-z||^2} = e^{-\pi||x-y||^2}$$



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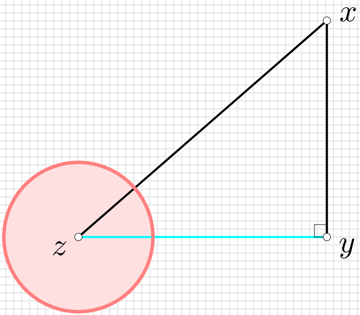
$$e^{-\pi||x-z||^2} = e^{-\pi||x-y||^2} e^{-\pi||y-z||^2}$$



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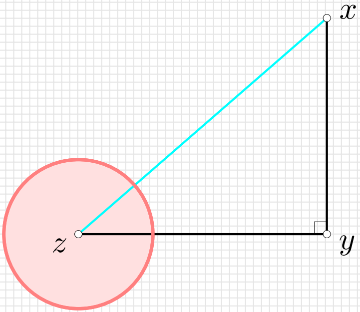
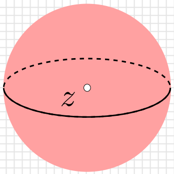
$$e^{-\pi||x-z||^2} = e^{-\pi||x-y||^2} e^{-\pi||y-z||^2}$$

$$||x - z||^2 = ||x - y||^2 + ||y - z||^2$$



Restrictions of Kernels



Restrictions of Kernels

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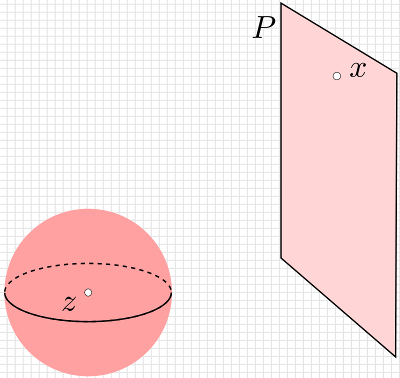
A *restriction* of g_z is the evaluation of the function on a lower-dimensional plane P.



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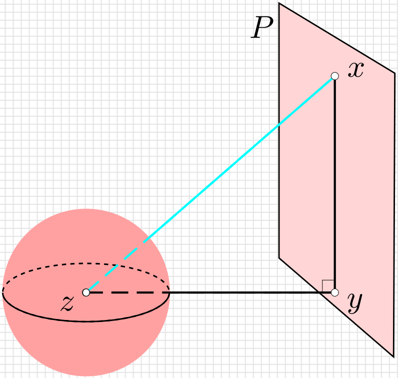
$$g_z|_P(x) = c_z g_y(x).$$



Gaussian Mixture

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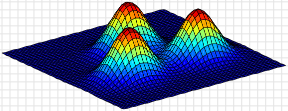

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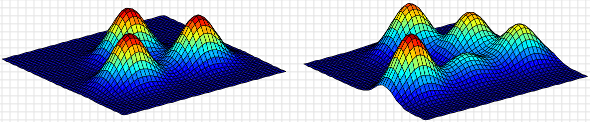

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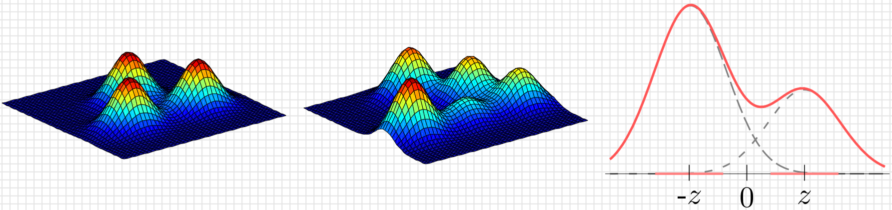
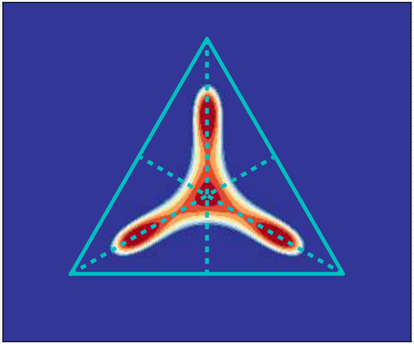
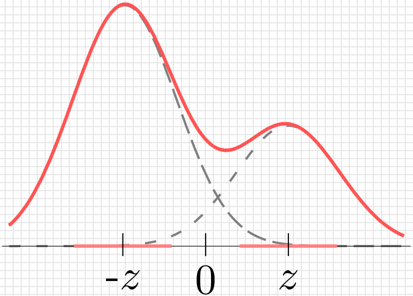


Restrictions of Mixtures





No Ghost Modes

Theorem

In $\mathbb{R}^1$, the number of modes is at most the number of components.

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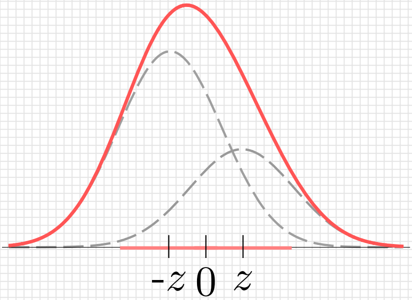
Question

When is the transition between having one mode and two?

Weighted Gaussian Mixture

$$G_w(x) = c_k g_{-z}(x) + c_\ell g_z(x).$$

Weighted Gaussian Mixture



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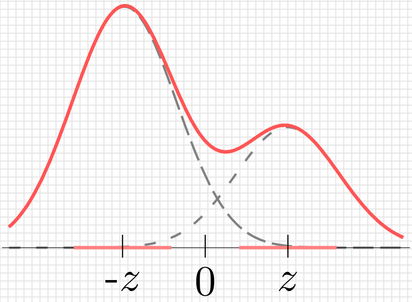
The Weighted Mixture

1. If z is small enough, then G_w has one critical point.

Weighted Gaussian Mixture



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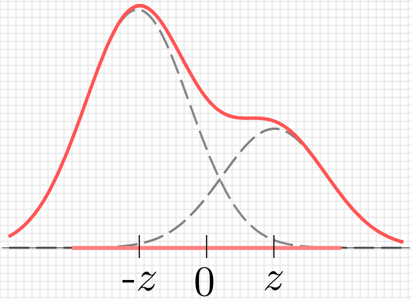

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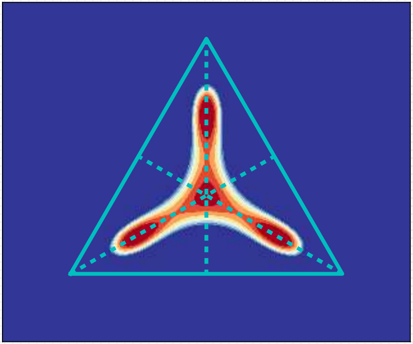
3. G_w has exactly 2 critical points when $\frac{c_k}{c_\ell} = r(x) + 1$.

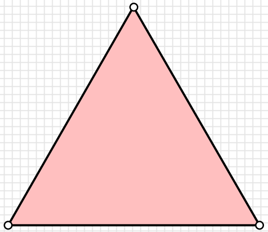
Counting Modes in $\mathbb{R}^n$

For $n \geq 2$, there can be more modes than components of a Gaussian mixture in $\mathbb{R}^n$.



Standard n-Simplex, Δ^n

An n-simplex is the convex hull of $n + 1$ vertices.



Standard n-Simplex, Δ^n

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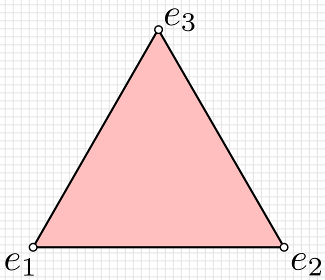
The *standard n-simplex* has the standard basis elements as the vertices:

$$e_1, e_2, \ldots, e_{n+1}.$$



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$\mathbb{R}^3$

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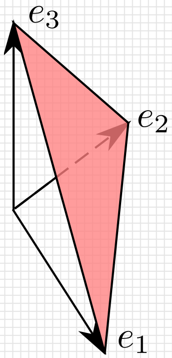

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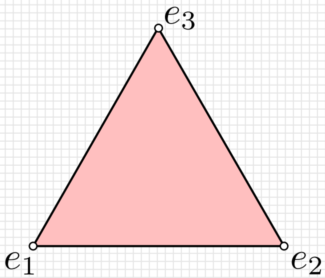
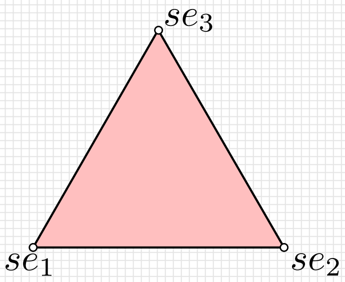


Scaled n-Simplex, $s\Delta^n$

$\mathbb{R}^3$

The *scaled standard n-simplex* in $\mathbb{R}^{n+1}$ is defined by the $n+1$ standard basis elements, scaled by a factor s

$$se_1, se_2, \ldots, se_{n+1}.$$



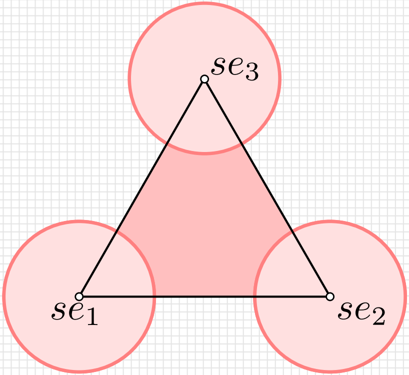
Scaled n-Design

$\mathbb{R}^3$

Definition

The *Scaled n-Design* is the Gaussian mixture with centers at the $n+1$ vertices of the scaled n-simplex:

$$G_s(x) = \sum_{i=1}^{n+1} g_{se_i}(x)$$



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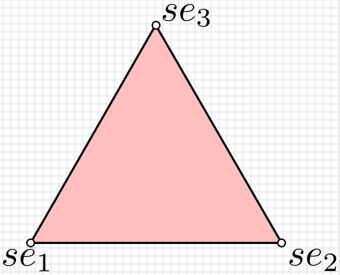

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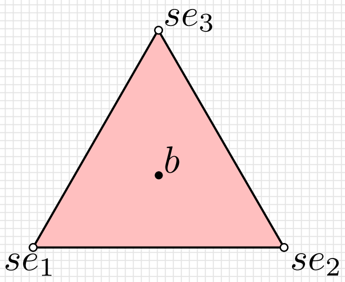
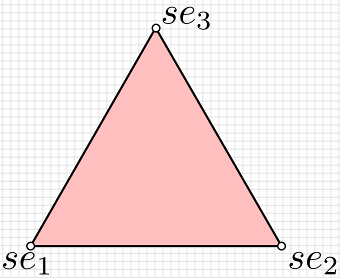
The *barycenter* is the average vertex position:

$$\left(\frac{s}{n+1}, \frac{s}{n+1}, \ldots, \frac{s}{n+1}\right).$$



Complementary Faces

$\mathbb{R}^3$



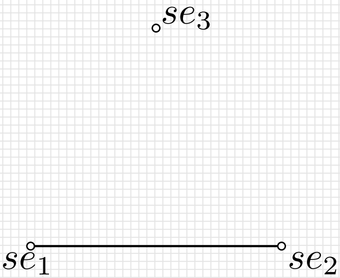
Complementary Faces

$\mathbb{R}^3$

We partition the vertices of the scaled n-simplex into two sets:

$$K = \{se_3\},$$
$$L = \{se_1, se_2\}.$$

Let $k = |K| - 1$ and $\ell = |L| - 1$.



Complementary Faces

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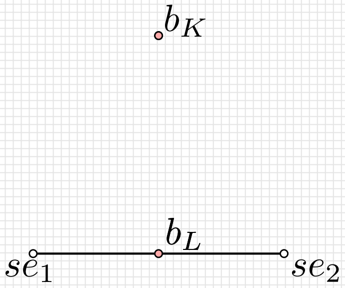
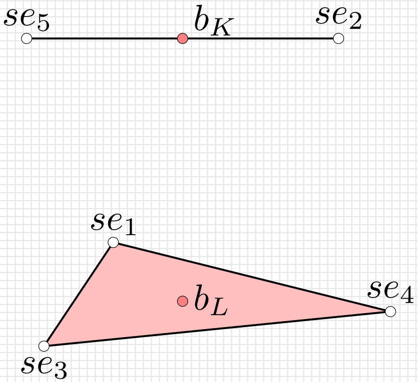


Complementary Faces

$\mathbb{R}^5$

We partition the vertices of the scaled *n*-simplex into two sets:

$$K = \{se_2, se_5\},$$
$$L = \{se_1, se_3, se_4\}.$$

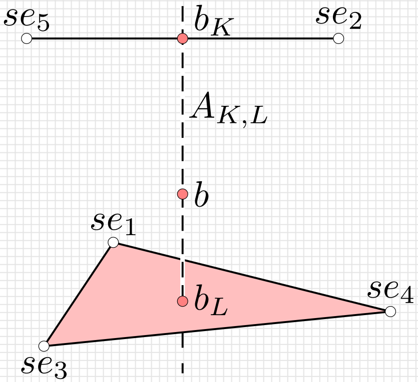


Let $k = |K| - 1$ and $\ell = |L| - 1$.

Location of Critical Points

$\mathbb{R}^5$

The axis $A_{K,L}$ is the line defined by b_K and b_L.



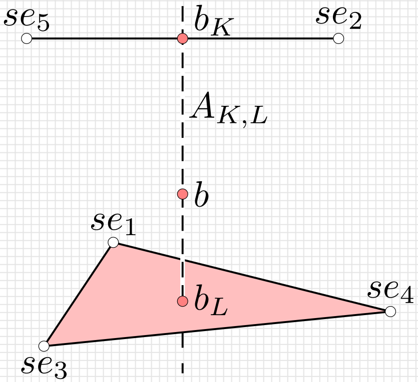
Location of Critical Points

$\mathbb{R}^5$

The axis $A_{K,L}$ is the line defined by b_K and b_L.

Location of Critical Values

All critical points of the scaled n-design lie on an axis of $s\Delta^n$.



Location of Critical Points

$\mathbb{R}^4$

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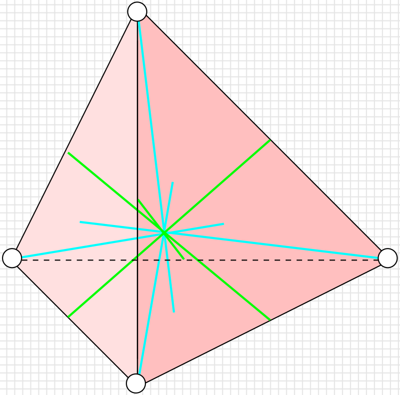

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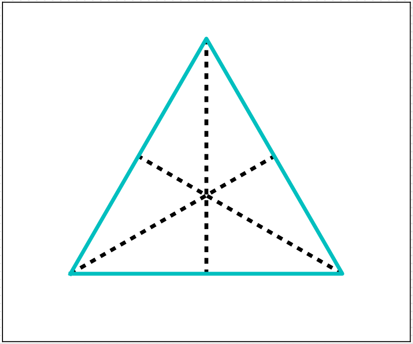

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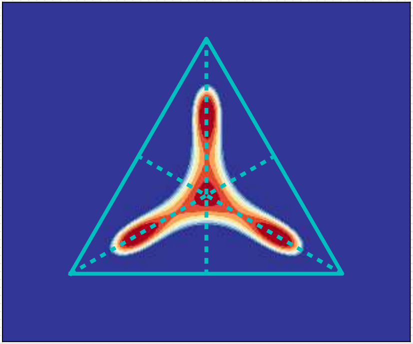

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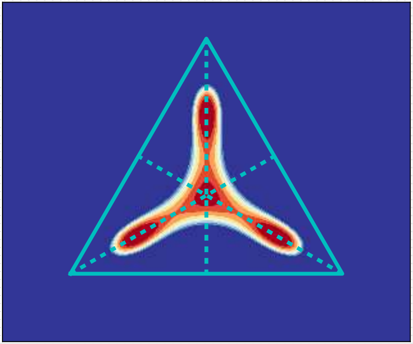
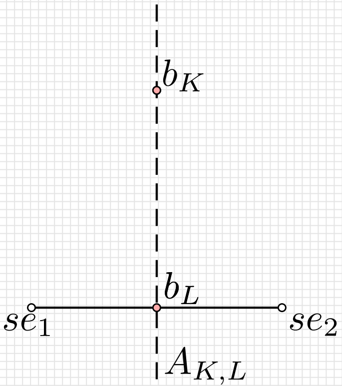
Proof

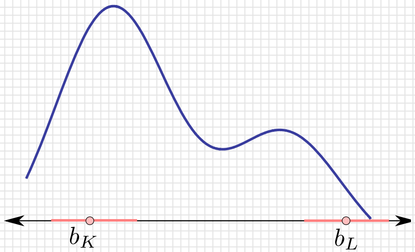
Assume a critical point x is not on an axis ...



Restriction to an Axis

$\mathbb{R}^3$





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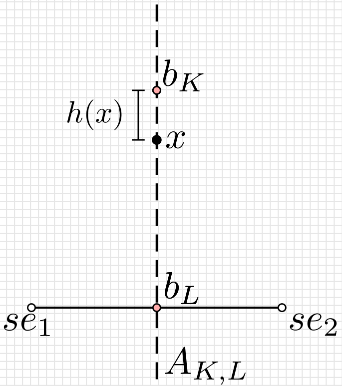

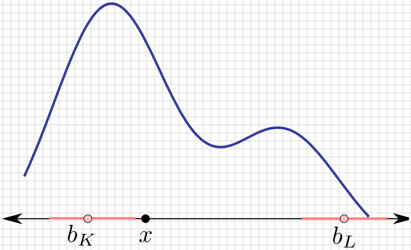

$$G_s|_A(x) = c_k e^{-\pi h(x)} + c_\ell e^{-\pi(D_{k,\ell} - h(x))},$$

where $c_k = (k+1) g_{se_i}(b_L), \quad c_\ell = (\ell+1) g_{se_j}(b_K).$

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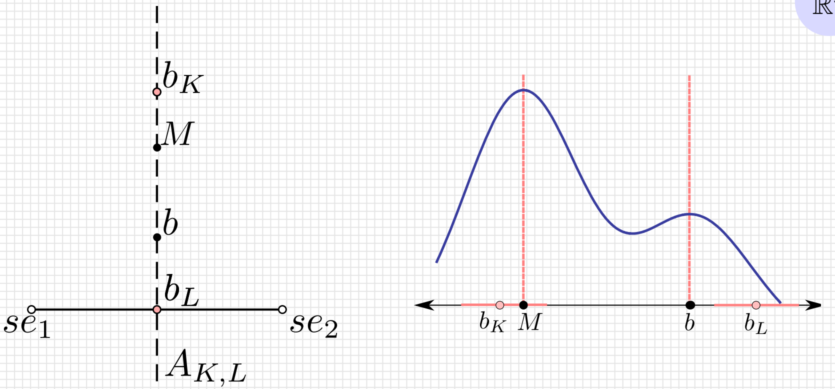

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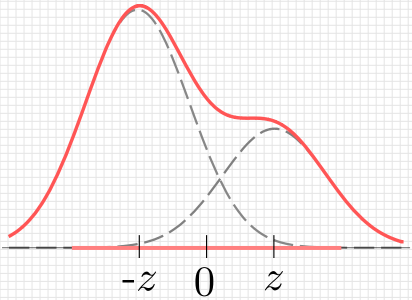
Weighted Gaussian Mixture



$$G_w(x) = c_k g_{-z}(x) + c_\ell g_z(x).$$

The Weighted Mixture

1. If z is small enough, then G_w has one critical point.
2. If z is large enough, then G_w has three critical points.
3. G_w has exactly 2 critical points when $\frac{c_k}{c_\ell} = r(x) + 1$.

Lower Transition Scale Factor $T_{k,\ell}$

Definition

$T_{k,\ell}$ is the scale factor for which

$$\frac{c_k}{c_\ell} = r(x) + 1.$$

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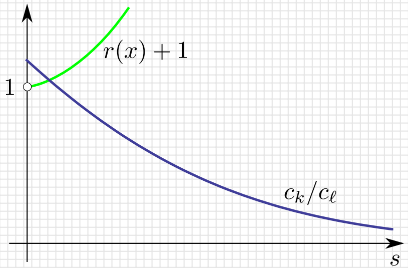

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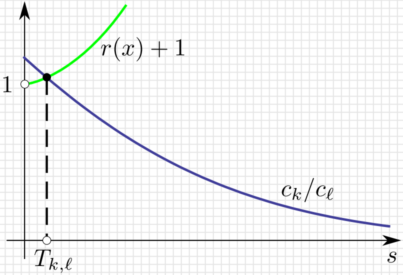

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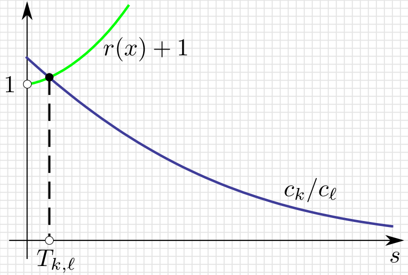
1-Dimensional Maxima Lemma

For all $s > T_{k,\ell}$, the axis $A_{K,L}$ witnesses two one-dimensional maxima.



Upper Transition Scale Factor U_n

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$$U_n = \sqrt{\frac{n+1}{2\pi}}.$$

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The barycenter of $s\Delta^n$ is a mode for $s < U_n$, and a saddle of index 1 for $s > U_n$.

One-Dimensional Maxima

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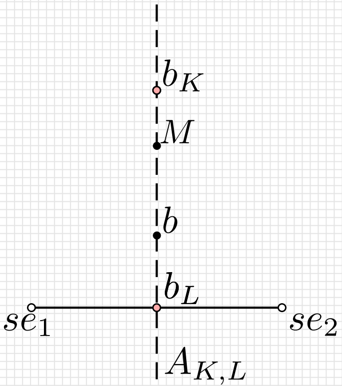
The barycenter of $s\Delta^n$ is a mode for $s < U_n$, and a saddle of index 1 for $s > U_n$.

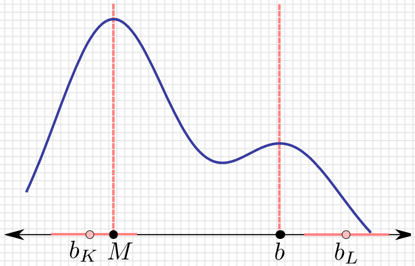
Theorem

If $s \in (T_{k,\ell}, U_n)$, then $A_{K,L}$ witnesses two one-dimensional maxima, one of which is at the barycenter.

Restriction to an Axis

$\mathbb{R}^5$





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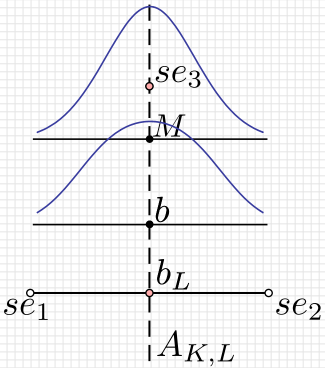
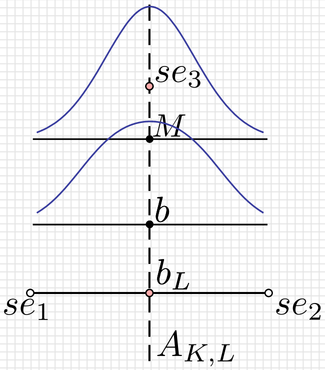
Witnessing the Modes



Witnessing the Modes



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If $|K| = 1$, then $A_{K,L}$ witnesses two modes for $s \in (T_{0,n-1}, U_n)$.

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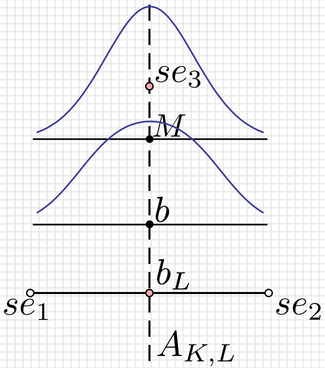

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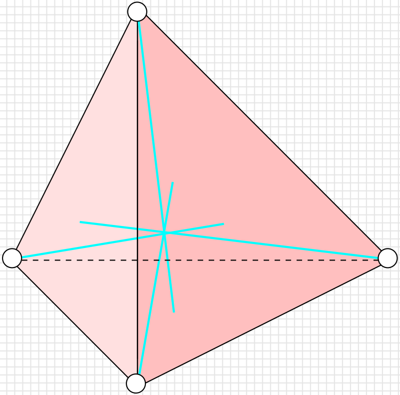
Witnessing Critical Points

If $|K| > 1$, then M is a critical point, not a mode.

Many Axes

$\mathbb{R}^4$

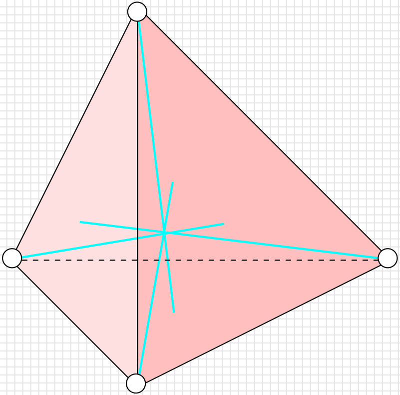


Many Axes

Number of Axes with $k = 0$:

$$n + 1.$$

$\mathbb{R}^4$



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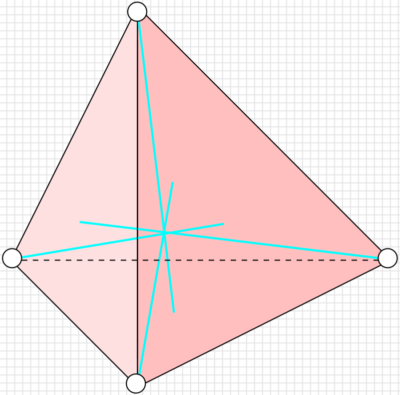

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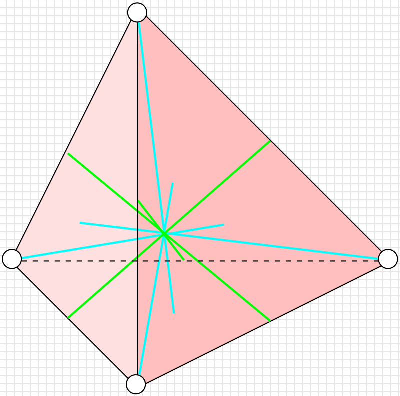

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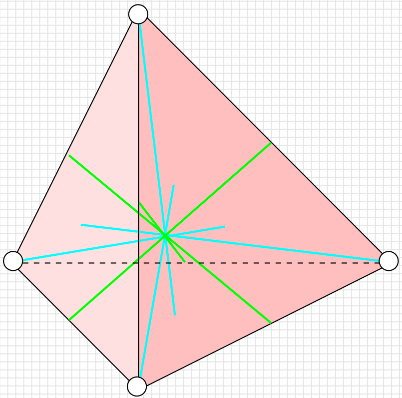
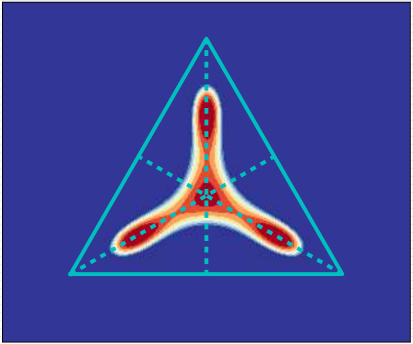
The scaled design has $\Theta(2^n)$ critical points.



$\mathbb{R}^4$

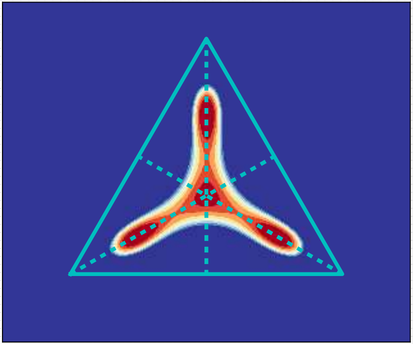
Summary of Results



Summary of Results

The *n*-design has:

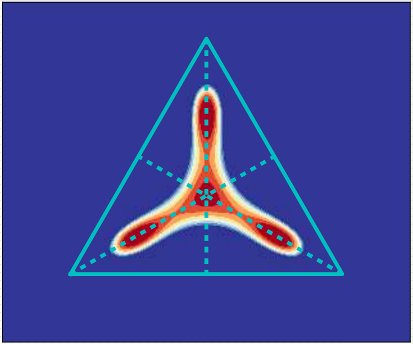
1. at most ONE ghost mode.



Summary of Results

The *n*-design has:

1. at most ONE ghost mode.
2. an exponential number of critical points.



Summary of Results

The *n*-design has:

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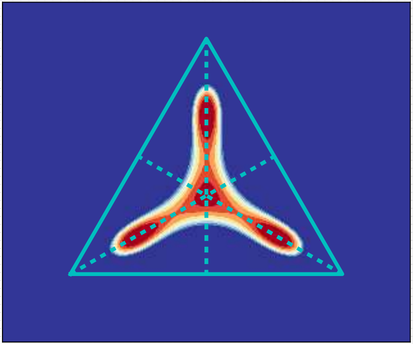

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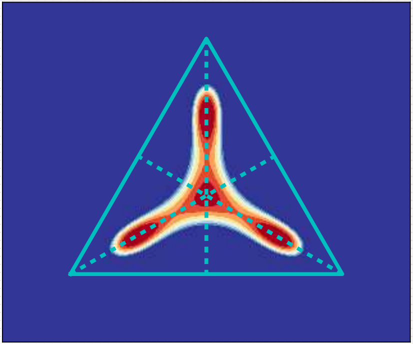
Wednesday at 2:50 in SN011:

1. How does $U_n - T_{0,n-1}$ (the resilience) grow with dimension?



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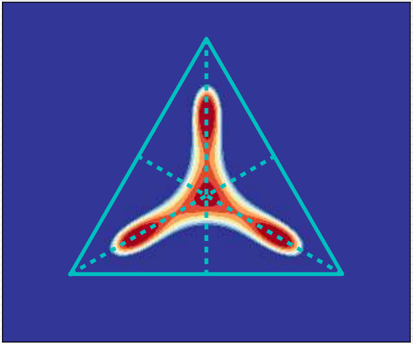

Add Isotropic Gaussian Kernels at Own Risk

More and More Resilient Modes in Higher Dimensions

Herbert Edelsbrunner, BRITTANY TERESE FASY, and Günter Rote

Symposium on Computational Geometry 2012
Chapel Hill, North Carolina

18 June 2012

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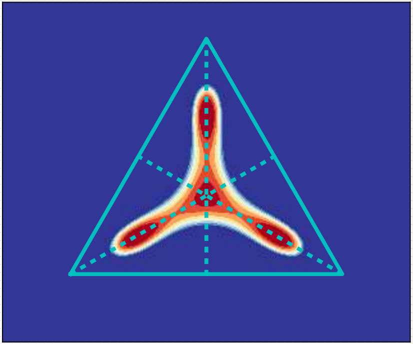

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