

Efficiently Learning Mixtures of Gaussians

Ankur Moitra, MIT

joint work with Adam Tauman Kalai and Gregory Valiant

May 11, 2010

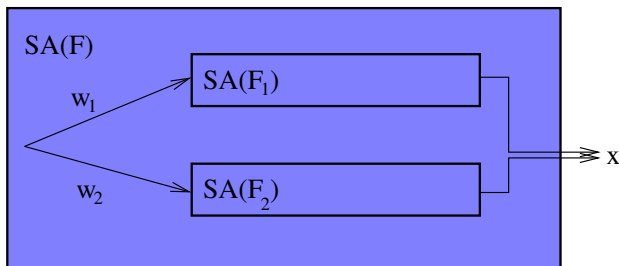
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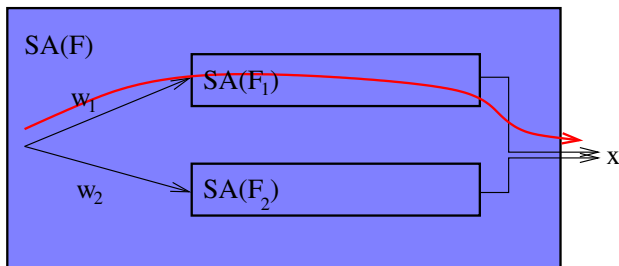
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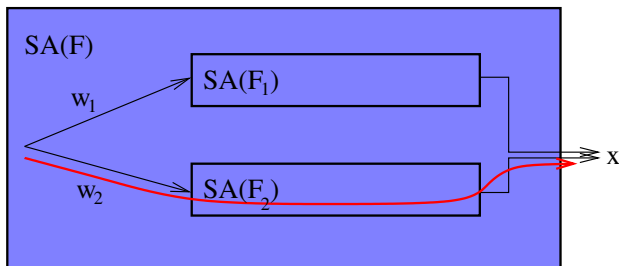
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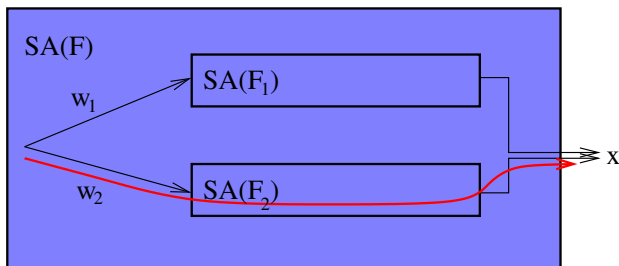
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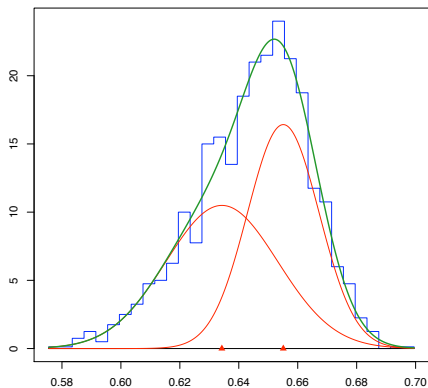
Distribution on \mathbb{R}^n ($w_1, w_2 \geq 0, w_1 + w_2 = 1$):



$$F(x) = w_1 \mathcal{N}(\mu_1, \Sigma_1, x) + w_2 \mathcal{N}(\mu_2, \Sigma_2, x)$$

Pearson and the Naples Crabs

(figure due to Peter Macdonald)



Let $F(x) = w_1 F_1(x) + w_2 F_2(x)$, where $F_i(x) = \mathcal{N}(\mu_i, \sigma_i^2, x)$

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Let $E_{x \leftarrow F_i(x)}[x^r] = M_r(\mu_i, \sigma_i^2)$

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What if we knew the r^{th} -raw moment of $F(x)$ **perfectly**?

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Definition

We will refer to $\tilde{M}_r = \frac{1}{|S|} \sum_{i \in S} x_i^r$ as the empirical r^{th} -raw moment of $F(x)$

Pearson's Sixth Moment Test

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- 3 This yields a list of candidate parameters $\vec{\theta}^a, \vec{\theta}^b, \dots$
- 4 Choose the candidate that is closest in sixth moment:

$$w_1 M_6(\mu_1, \sigma_1^2) + (1 - w_1) M_6(\mu_2, \sigma_2^2) \approx \tilde{M}_6$$

"Given the probable error of every ordinate of a frequency-curve, what are the probable errors of the elements of the two normal curves into which it may be dissected?" [Karl Pearson]

Question

How does noise in the empirical moments translate to noise in the derived parameters?

Gaussian Mixture Models

Applications in physics, biology, geology, social sciences ...

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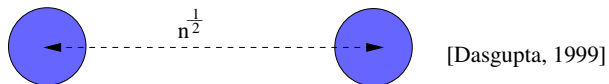
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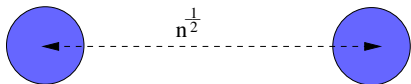
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$$D(f(x), g(x)) = \frac{1}{2} \|f(x) - g(x)\|_1$$

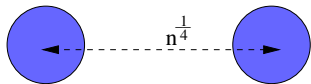
A History of Learning Mixtures of Gaussians



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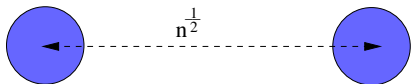


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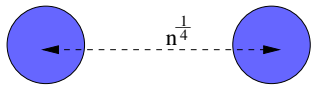


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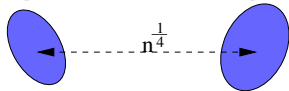
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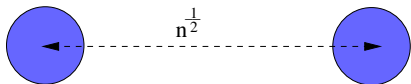


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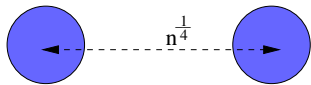


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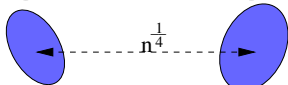
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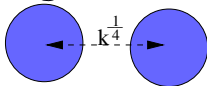
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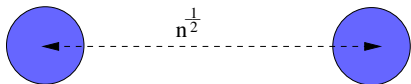


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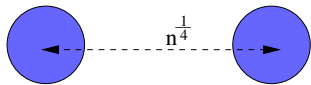


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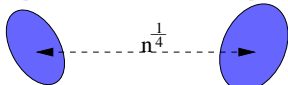
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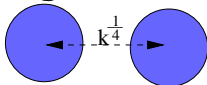
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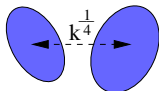
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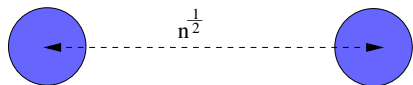


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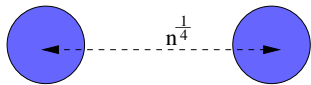


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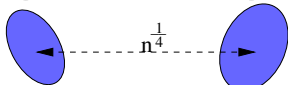
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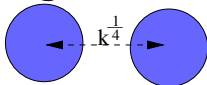
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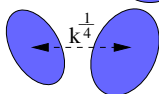
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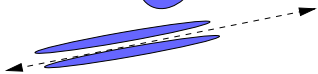
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[Brubaker, Vempala, 2008]

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Can we learn the parameters of the mixture without clustering?

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*Can we learn the parameters when $D(F_1, F_2)$ is close to **ZERO**?*

Goal

Learn a mixture $\hat{F} = \hat{w}_1 \hat{F}_1 + \hat{w}_2 \hat{F}_2$ so that there is a permutation $\pi : \{1, 2\} \rightarrow \{1, 2\}$ and for $i = \{1, 2\}$

$$|w_i - \hat{w}_{\pi(i)}| \leq \epsilon, D(F_i, \hat{F}_{\pi(i)}) \leq \epsilon$$

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When can we hope to learn an ϵ -close estimate?

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Definition

A mixture of Gaussians $F = w_1 F_1 + w_2 F_2$ is ϵ -statistically learnable if for $i \in \{1, 2\}$, $w_i \geq \epsilon$ and $D(F_1, F_2) \geq \epsilon$.

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Given oracle access to an ϵ -statistically learnable mixture of two Gaussians F :

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Given oracle access to an ϵ -statistically learnable mixture of two Gaussians F :

Theorem (Kalai, M, Valiant)

There is an algorithm that (with probability at least $1 - \delta$) learns a mixture of two Gaussians \hat{F} that is an ϵ -close estimate to F , and the running time and data requirements are $\text{poly}(\frac{1}{\epsilon}, n, \frac{1}{\delta})$.

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Previously, even no inverse exponential estimator known for univariate mixtures of two Gaussians

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A mixture of k Gaussians $F = \sum_i w_i F_i$ is ϵ -statistically learnable if for $i = \{1, 2, \dots, k\}$, $w_i \geq \epsilon$ and for all i, j $D(F_i, F_j) \geq \epsilon$.

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Definition

An estimate $\hat{F} = \sum_i \hat{w}_i \hat{F}_i$ mixture of k Gaussians is ϵ -close to F if there is a permutation $\pi : \{1, 2, \dots, k\} \rightarrow \{1, 2, \dots, k\}$ and for $i = \{1, 2, \dots, k\}$

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Corollary: First polynomial time density estimation for mixtures of Gaussians **with no assumptions!**

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A distribution $F(x)$ is in isotropic position if

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- 2 $E_{x \leftarrow F(x)}[(u^T x)^2] = 1$ for all $\|u\| = 1$

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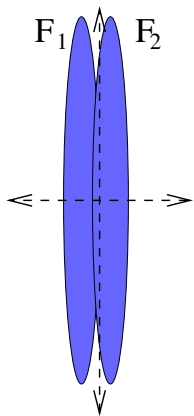
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Fact

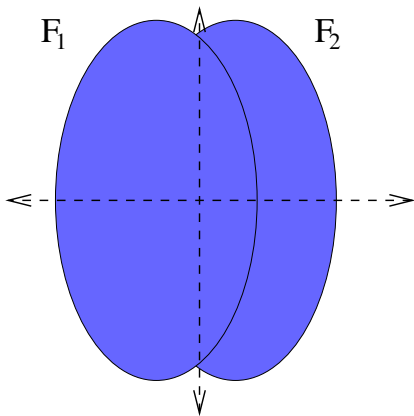
For any distribution $F(x)$ on \mathfrak{R}^n , there is an affine transformation T that places $F(x)$ in isotropic position

Isotropic Position

Not Isotropic



Isotropic



Given

Mixture F of two Gaussians, ϵ -statistically learnable, and in isotropic position

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Output

$$\hat{F} = \hat{w}_1 \hat{F}_1 + \hat{w}_2 \hat{F}_2 \text{ s.t.}$$

$$|w_i - \hat{w}_{\pi(i)}|, \|\mu_i - \hat{\mu}_{\pi(i)}\|, \|\Sigma_i - \hat{\Sigma}_{\pi(i)}\|_F \leq \epsilon$$

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- 1 Consider a series of projections down to one dimension

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Rough Idea

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- 2 Run a univariate learning algorithm
- 3 Use these estimates as constraints in a system of equations
- 4 Solve this system to obtain higher dimensional estimates

Claim

$$\text{Proj}_r[F_1] = \mathcal{N}(r^T \mu_1, r^T \Sigma_1 r, x)$$

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Definition

$$D_p(\mathcal{N}(\mu_1, \sigma_1^2), \mathcal{N}(\mu_2, \sigma_2^2)) = |\mu_1 - \mu_2| + |\sigma_1^2 - \sigma_2^2|$$

Problem

What if we choose a direction r s.t. $D_p(\text{Proj}_r[F_1], \text{Proj}_r[F_2])$ is extremely small?

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What if we choose a direction r s.t. $D_p(\text{Proj}_r[F_1], \text{Proj}_r[F_2])$ is extremely small?

Then we would need to run the univariate algorithm with extremely fine precision!

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(i.e. at least $\text{poly}(\epsilon, \frac{1}{n})$)

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Suppose $F = w_1 F_1 + w_2 F_2$ is in isotropic position and is ϵ -statistically learnable:

Isotropic Projection Lemma

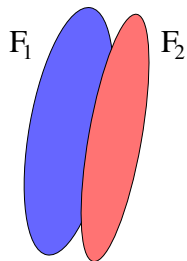
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Lemma (Isotropic Projection Lemma)

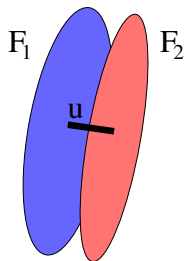
With probability $\geq 1 - \delta$ over a randomly chosen direction r ,

$$D_p(\text{Proj}_r[F_1], \text{Proj}_r[F_2]) \geq \frac{\epsilon^5 \delta^2}{50n^2} = \epsilon_3.$$

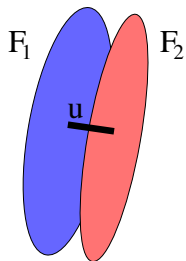
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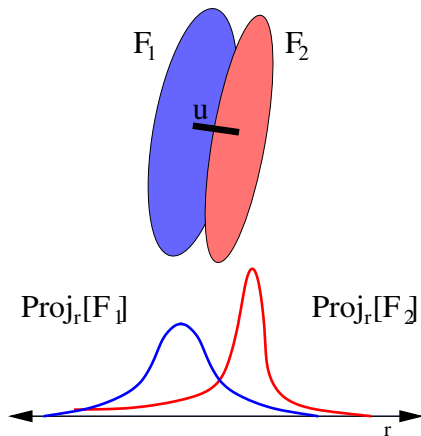
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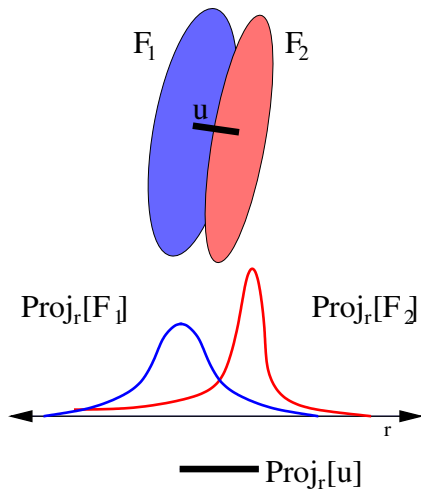
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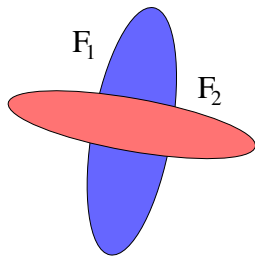
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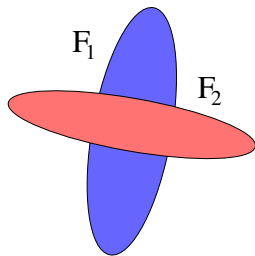
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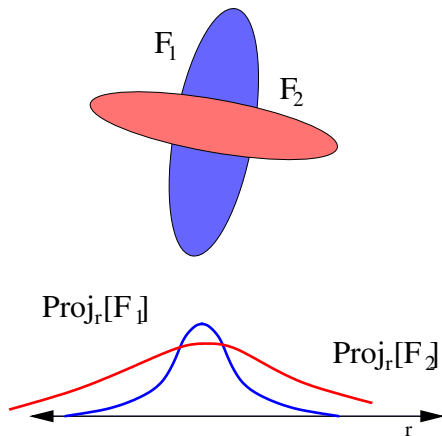
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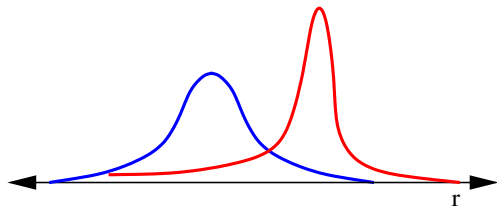
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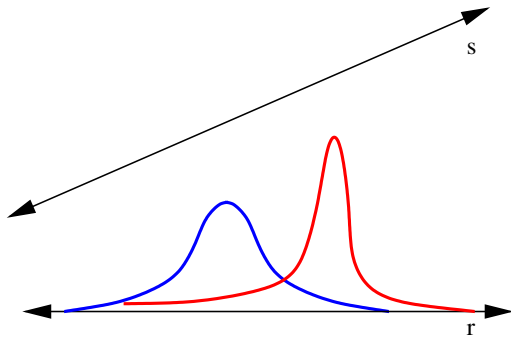
Problem

*How do we know that they yield constraints on the **SAME** Gaussian?*

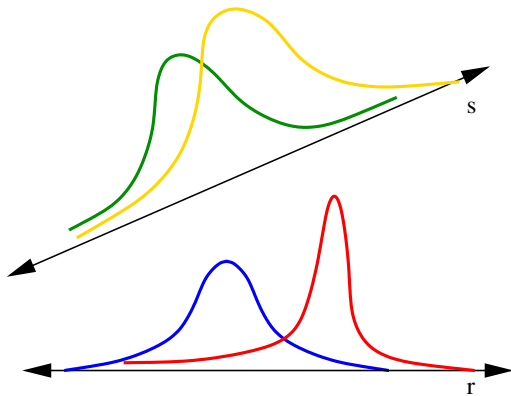
Searching Nearby Directions



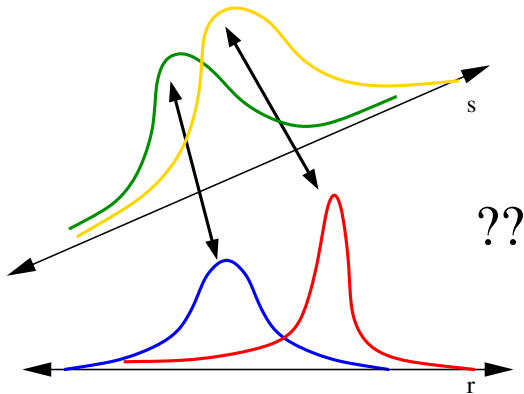
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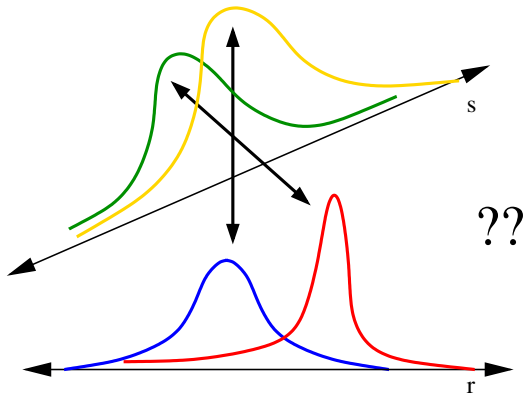
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("close enough" depends on the **Isotropic Projection Lemma**)

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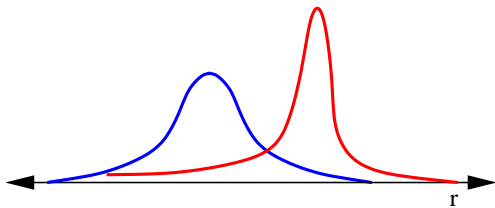
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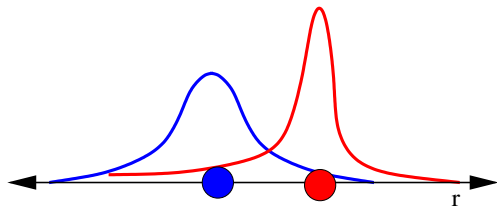
Lemma (Pairing Lemma)

$$D_p(\text{Proj}_r[F_i], \text{Proj}_s[F_i]) \leq O\left(\frac{\epsilon_2}{\epsilon}\right) \ll \frac{\epsilon_3}{3}$$

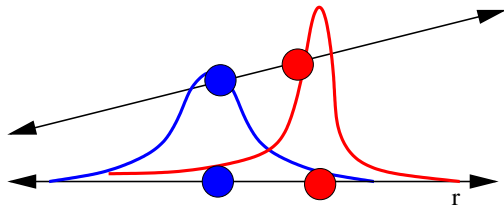
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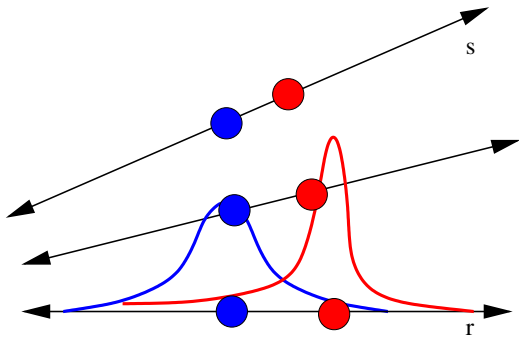
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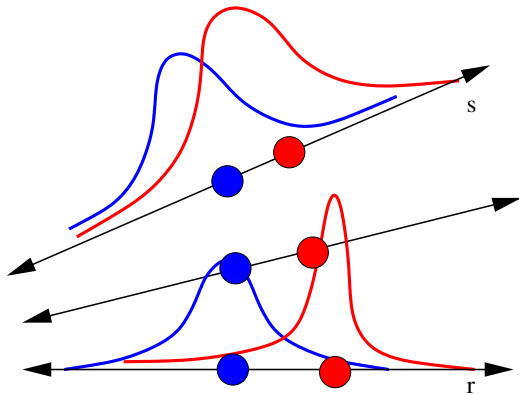
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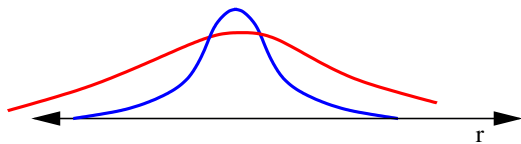
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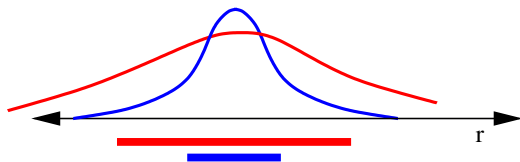
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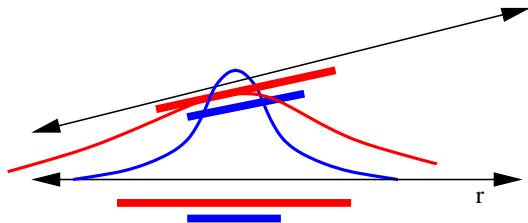
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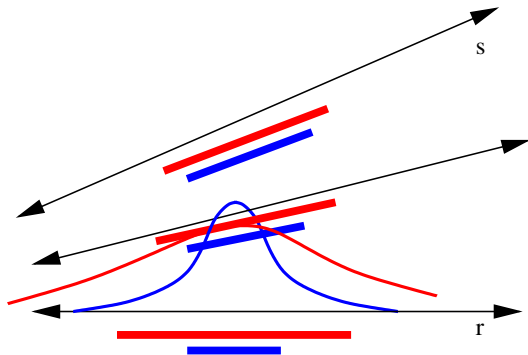
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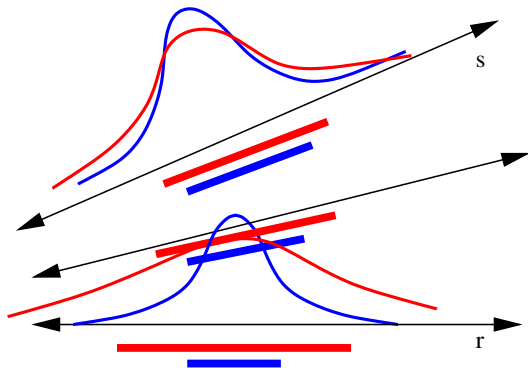
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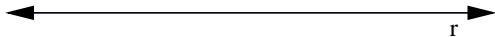
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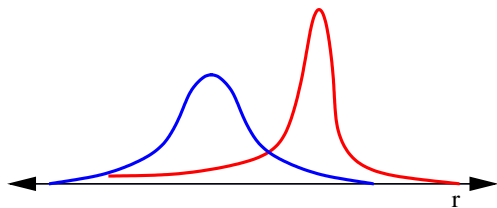
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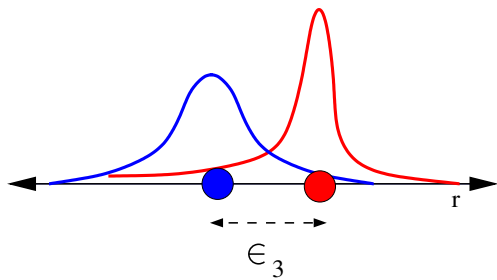
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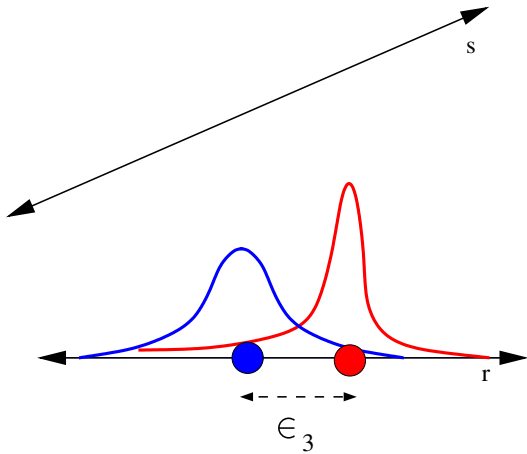
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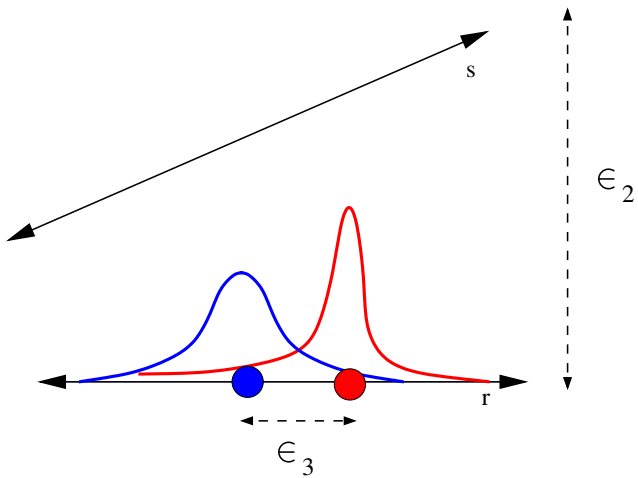
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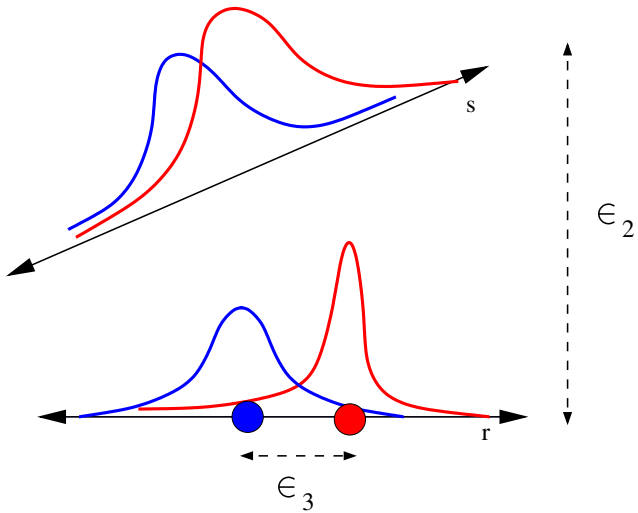


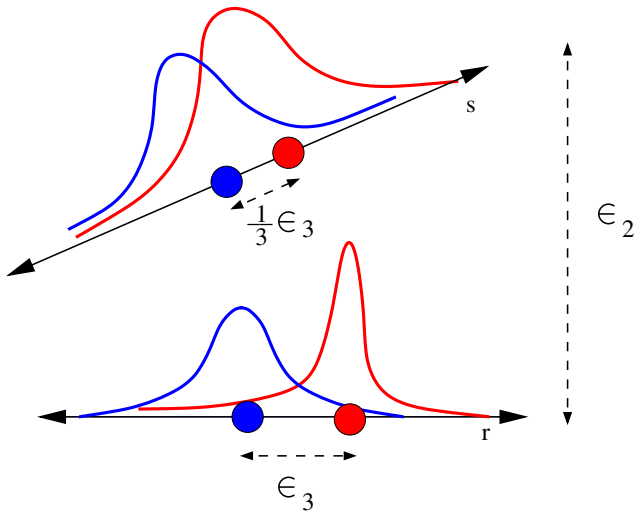


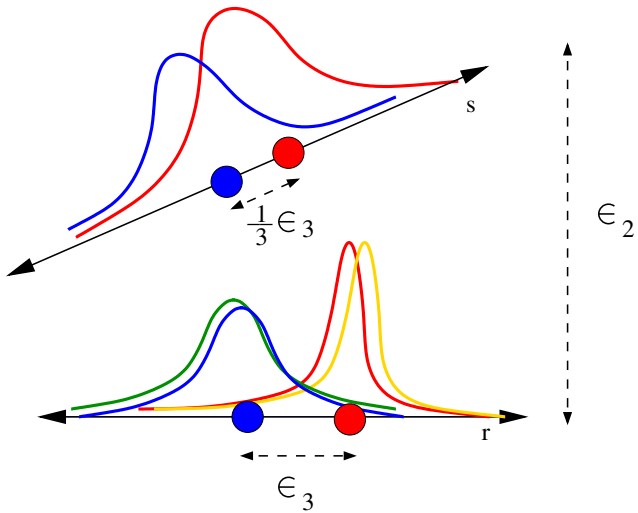


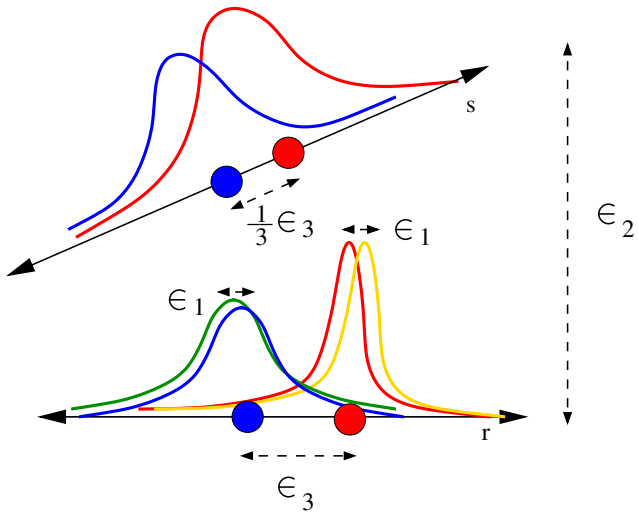


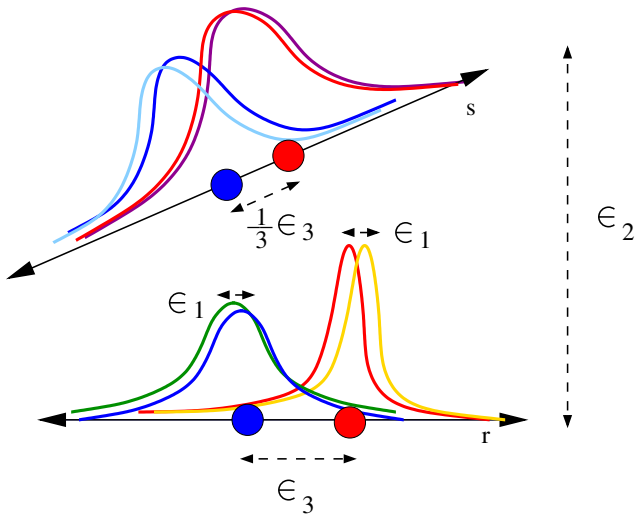


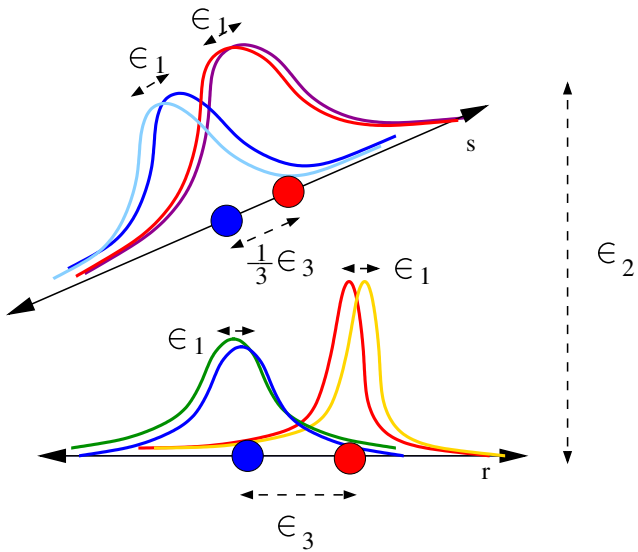


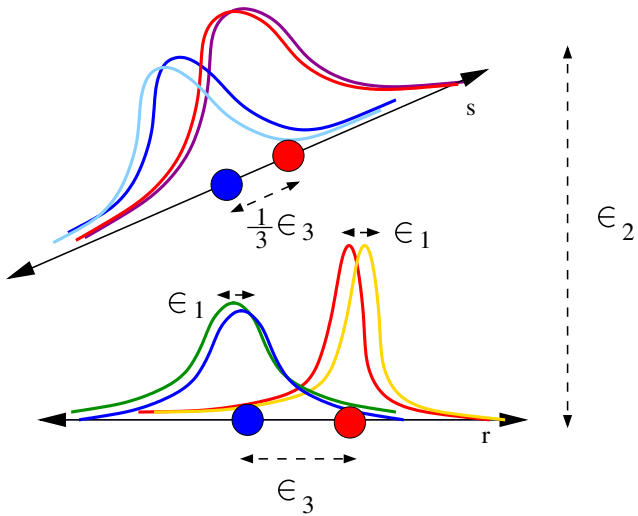


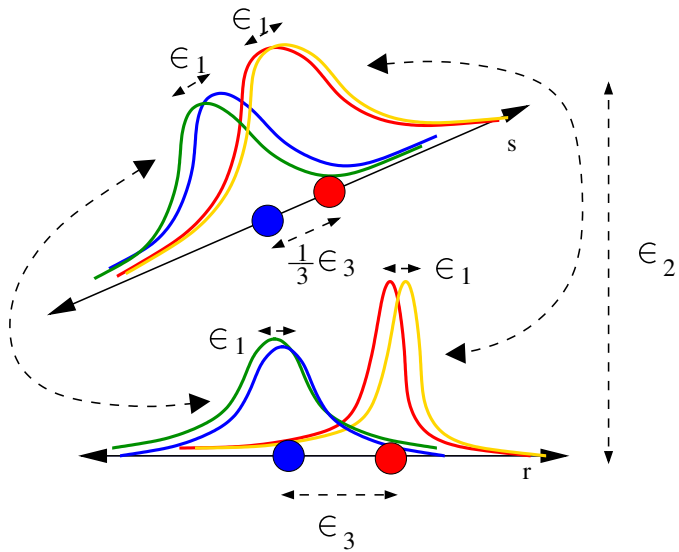


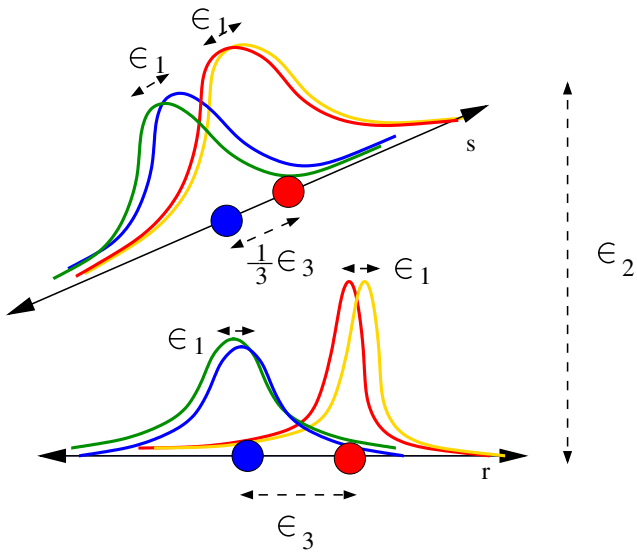


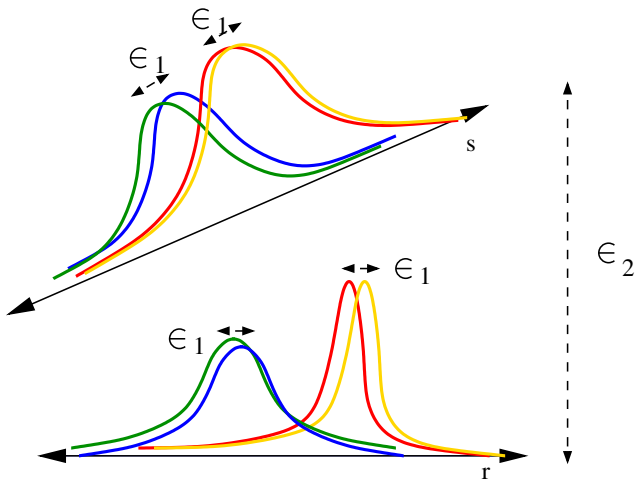


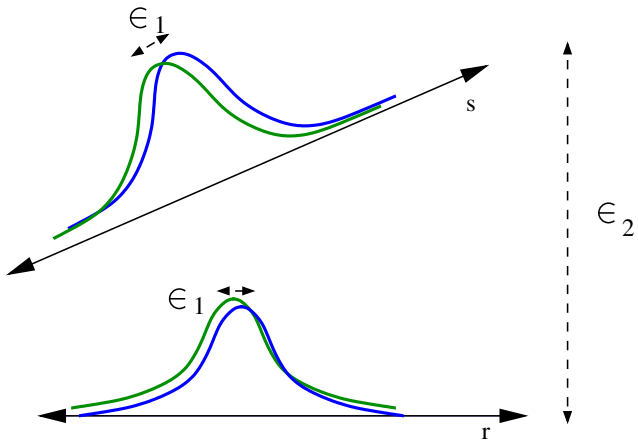


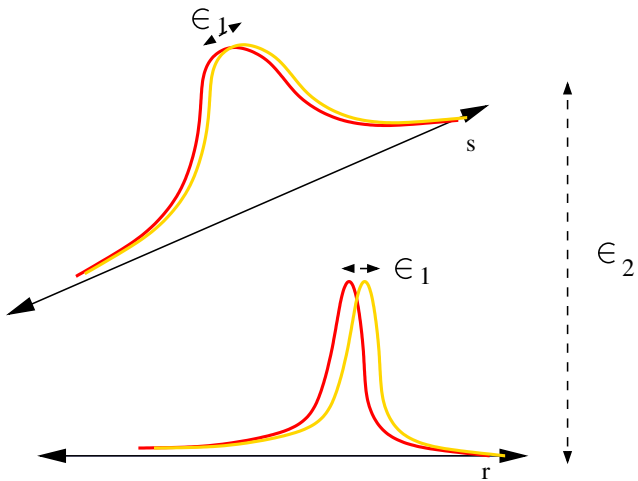










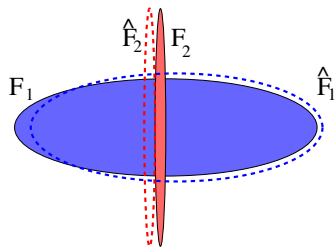


$SA(\tilde{F})$

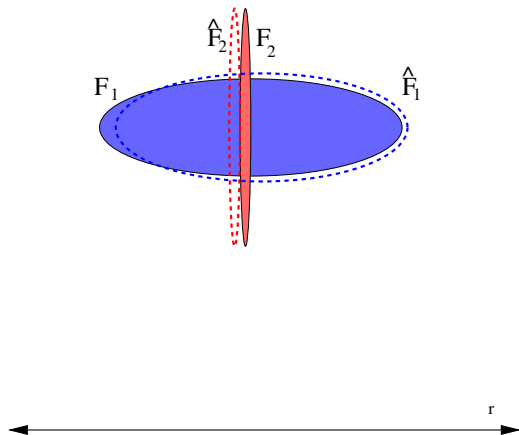
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graph TD; A[SA(F-tilde)] --> B[Additive Isotropic];
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Additive Isotropic

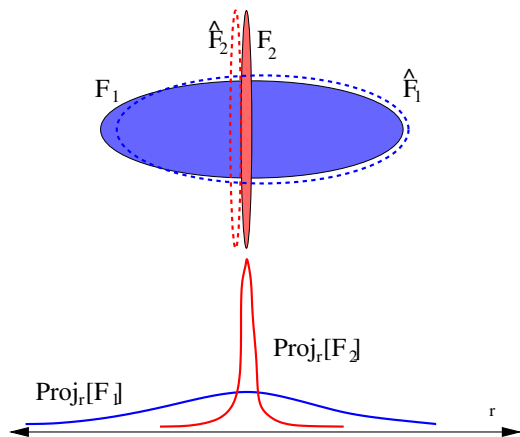
Using Additive Estimates to Cluster



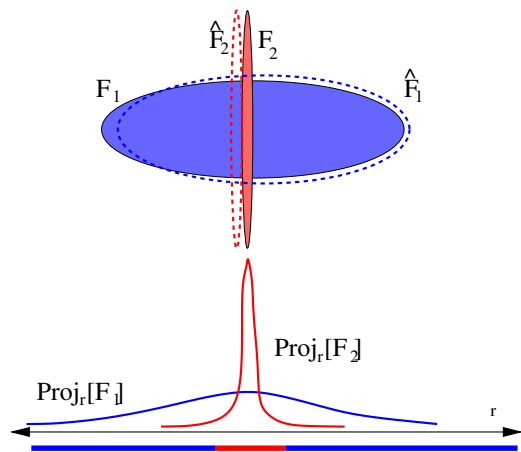
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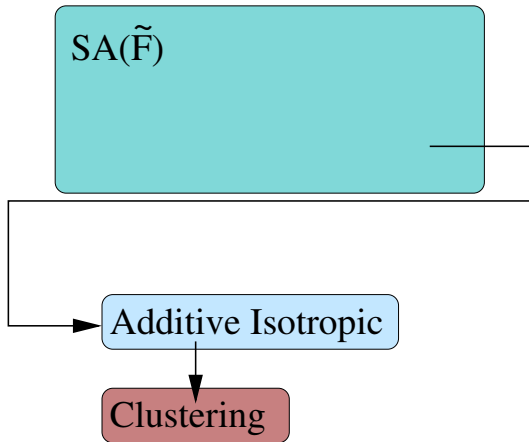
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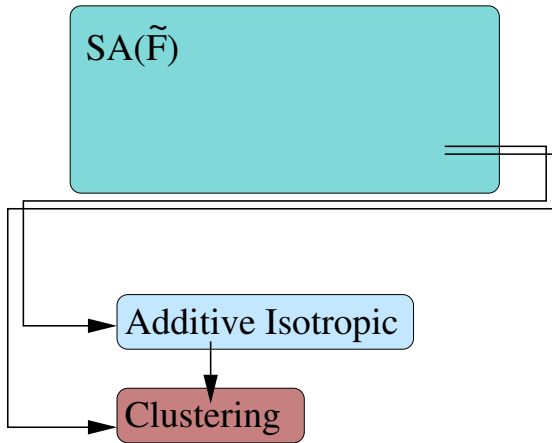


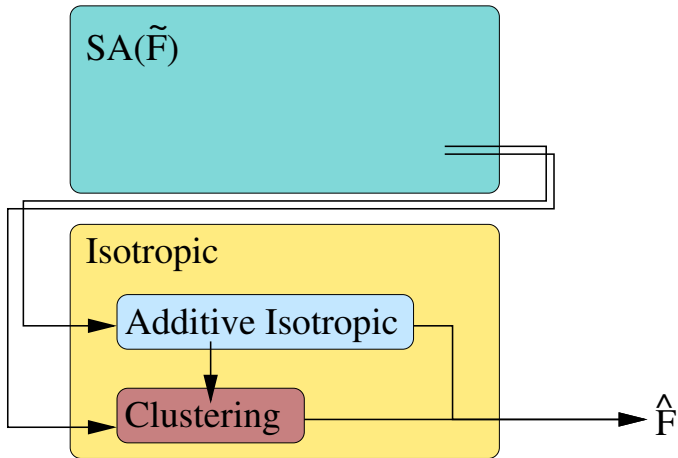
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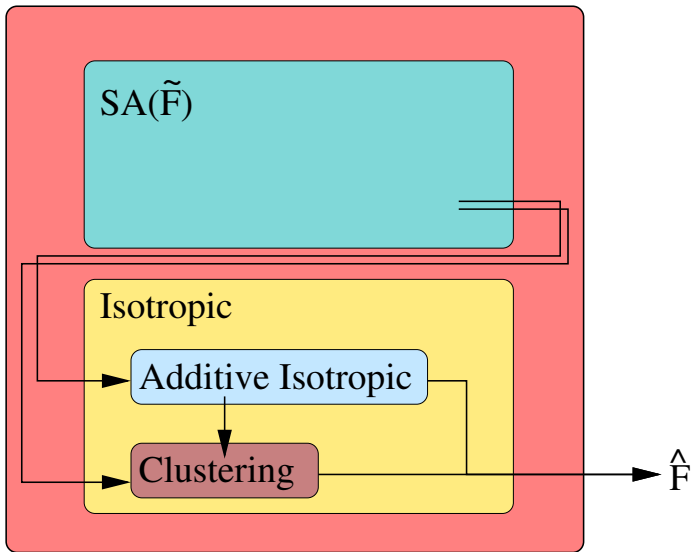
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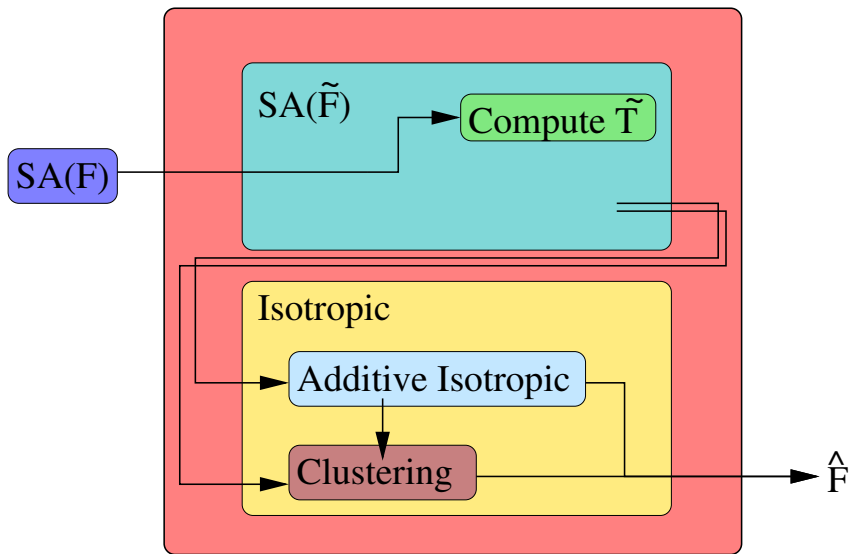


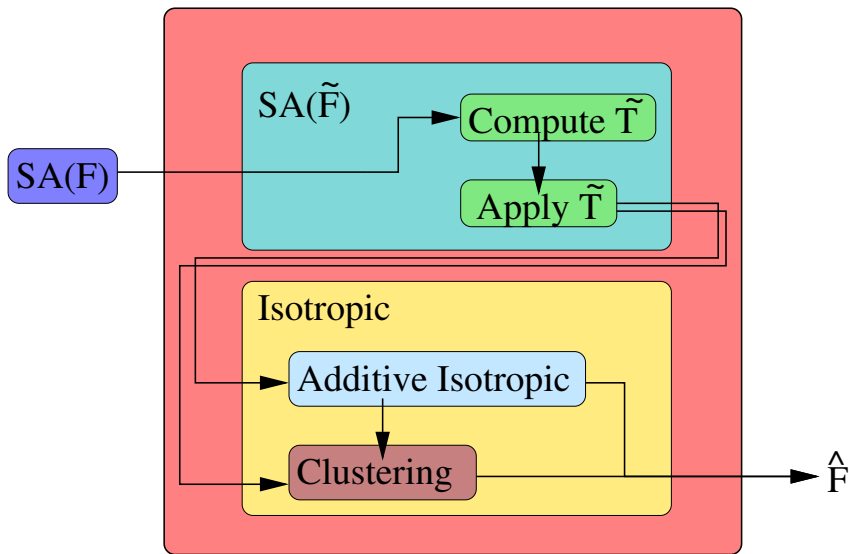


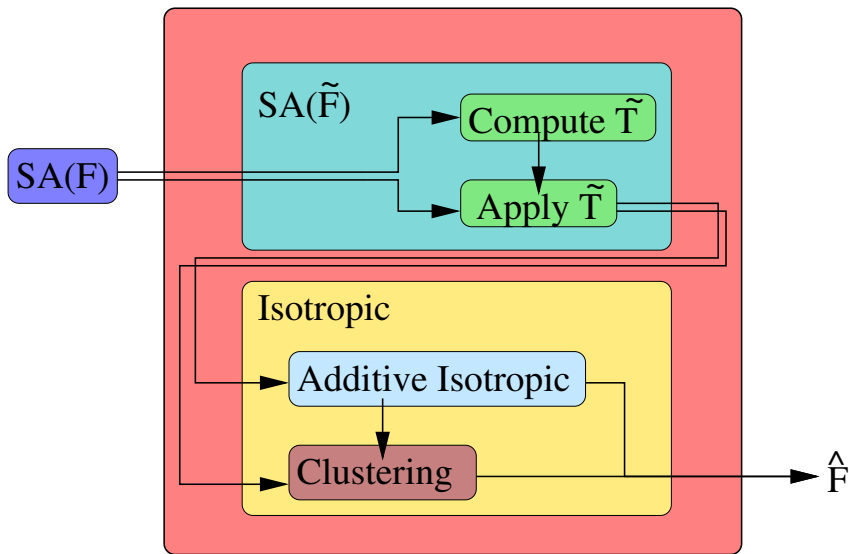


SA(F)









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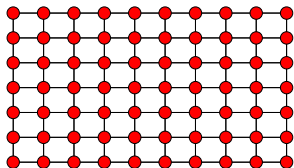
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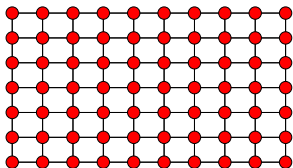
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In this case, we call the parameters ϵ -bounded

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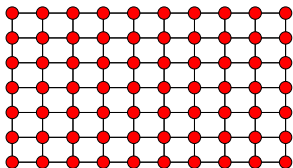
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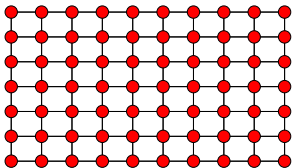


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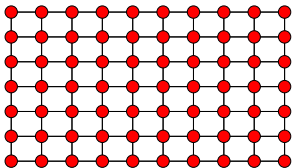


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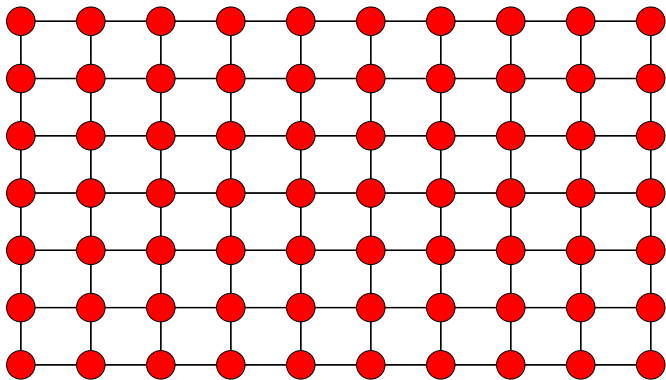
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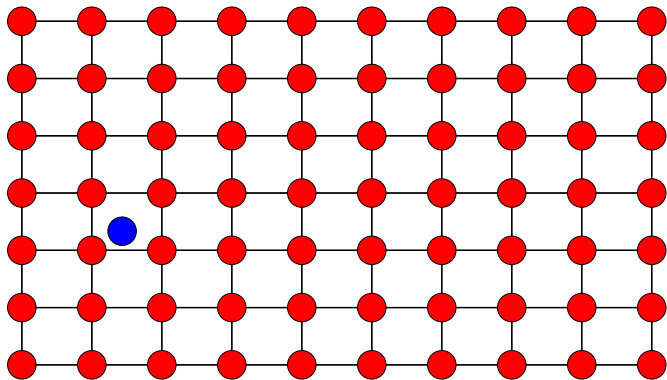


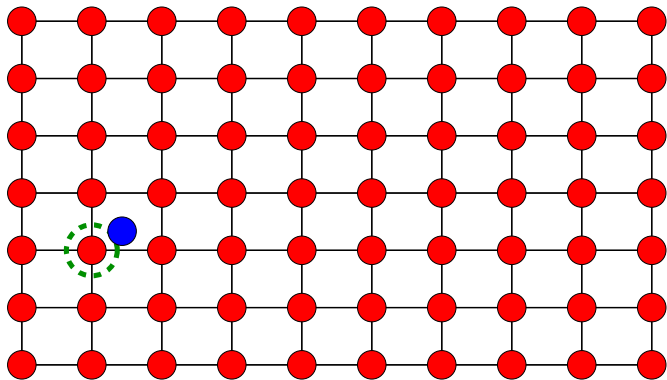
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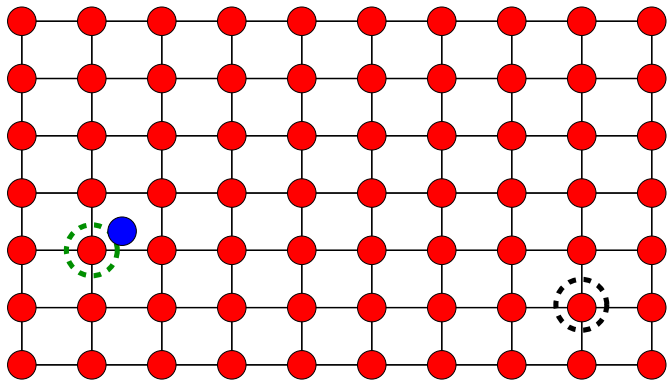
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- 3 Accept if $\tilde{M}_r \approx M_r(\hat{F})$ for all $r \in \{1, 2, \dots, 6\}$









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The pair F, \hat{F} ϵ -standard if

- 1 the parameters of F, \hat{F} are ϵ -bounded

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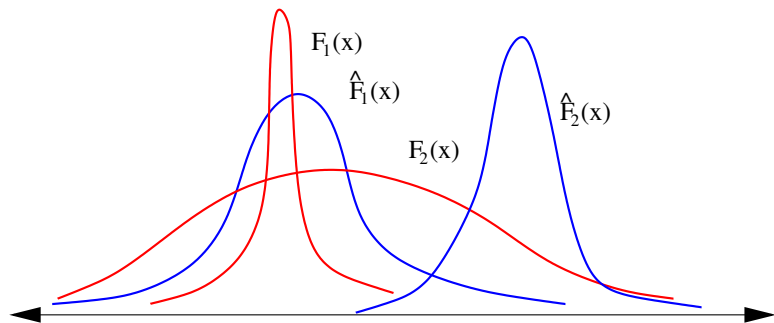
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Theorem

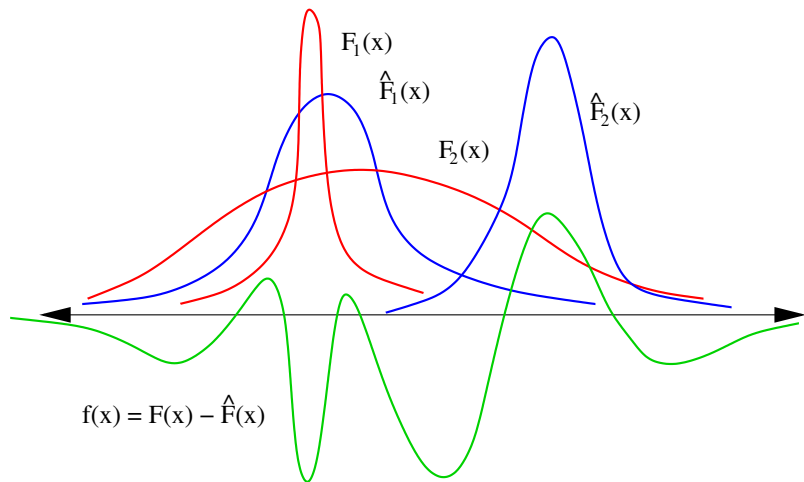
There is a constant $c > 0$ such that, for any any $\epsilon < c$ and any ϵ -standard F, \hat{F} ,

$$\max_{r \in \{1, 2, \dots, 6\}} |M_r(F) - M_r(\hat{F})| \geq \epsilon^{67}$$

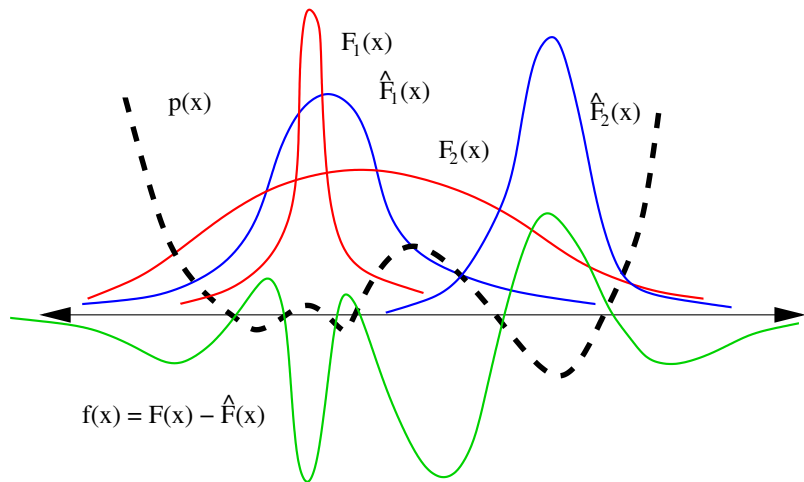
Method of Moments



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So $\exists_{r \in \{1,2,\dots,6\}}$ s.t. $|M_r(F) - M_r(\hat{F})| > 0$

Proposition

Let $f(x) = \sum_{i=1}^k \alpha_i \mathcal{N}(\mu_i, \sigma_i^2, x)$ be a linear combination of k Gaussians (α_i can be negative). Then if $f(x)$ is not identically zero, $f(x)$ has at most $2k - 2$ zero crossings.

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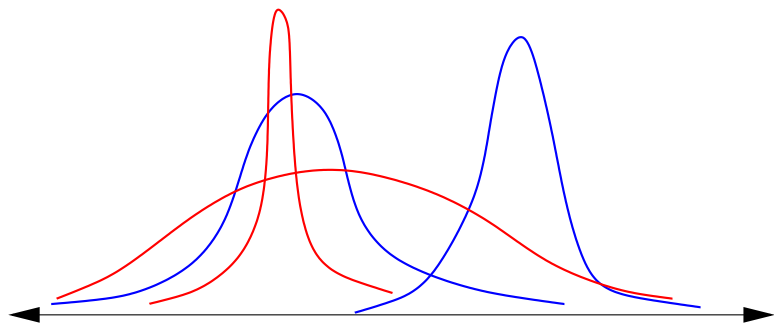
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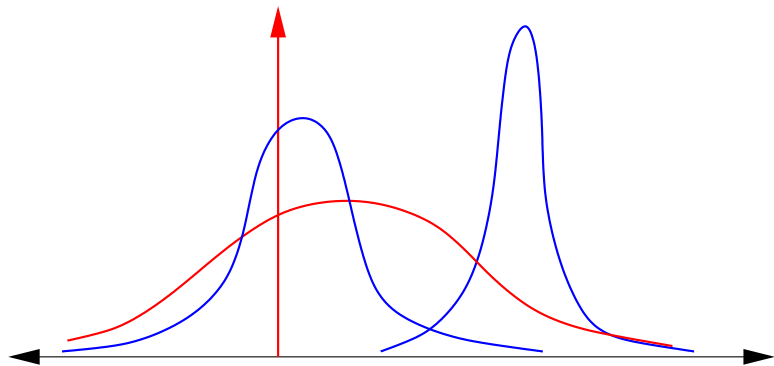
Fact

$$\mathcal{N}(0, \sigma_1^2, x) \circ \mathcal{N}(0, \sigma_2^2, x) = \mathcal{N}(0, \sigma_1^2 + \sigma_2^2, x)$$

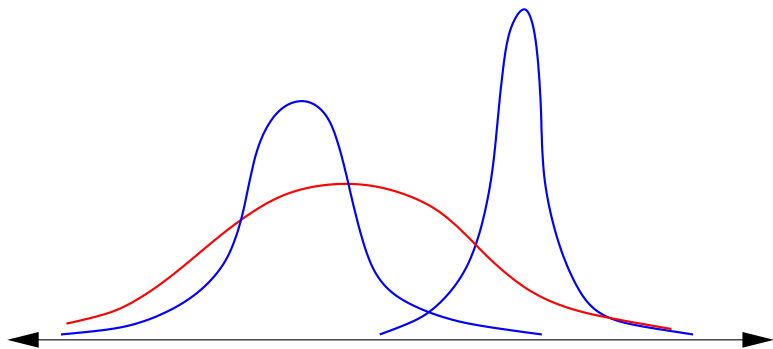
Zero Crossings and the Heat Equation



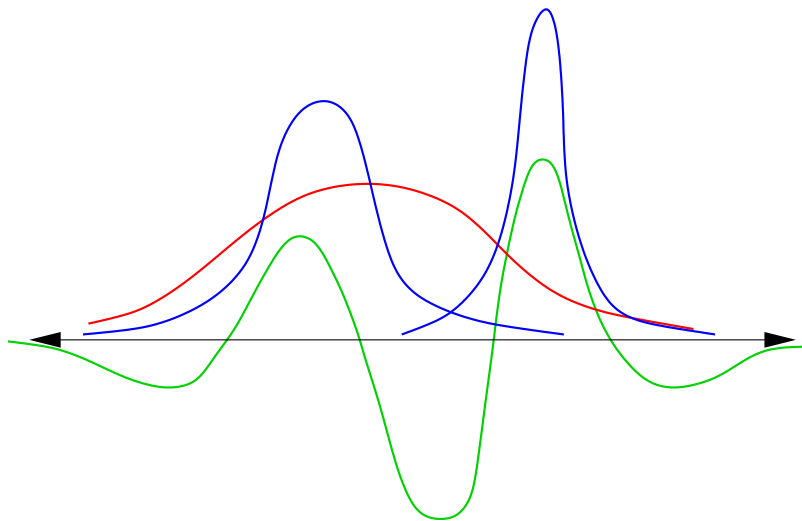
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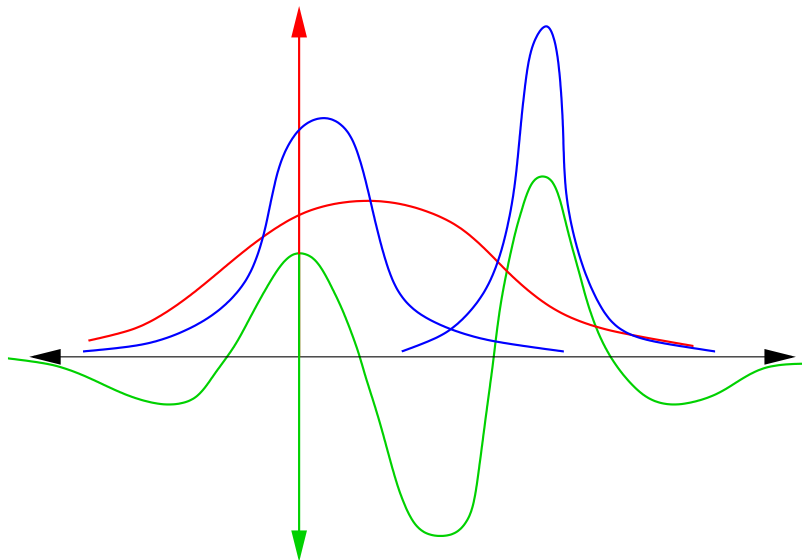
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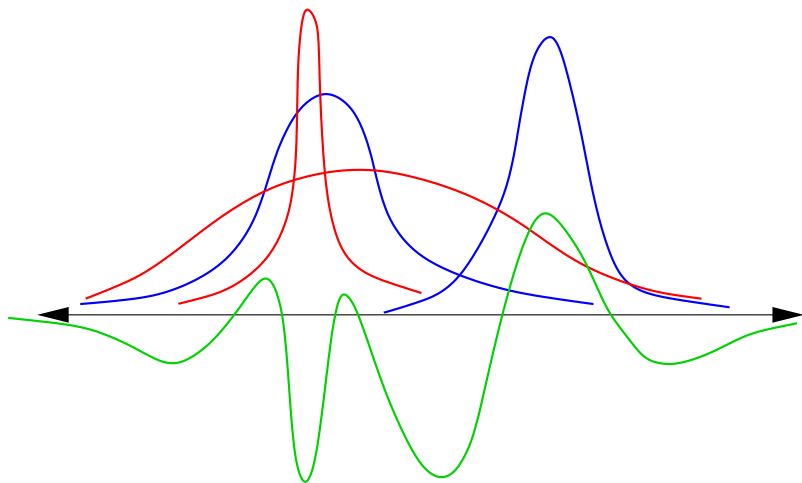
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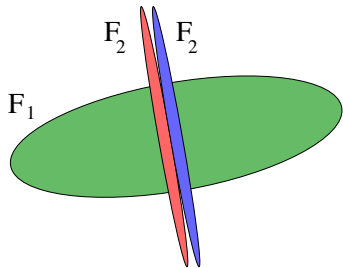


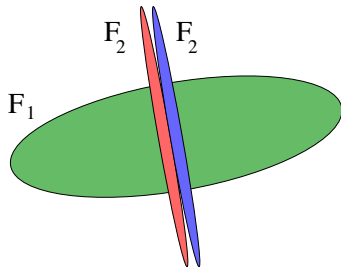
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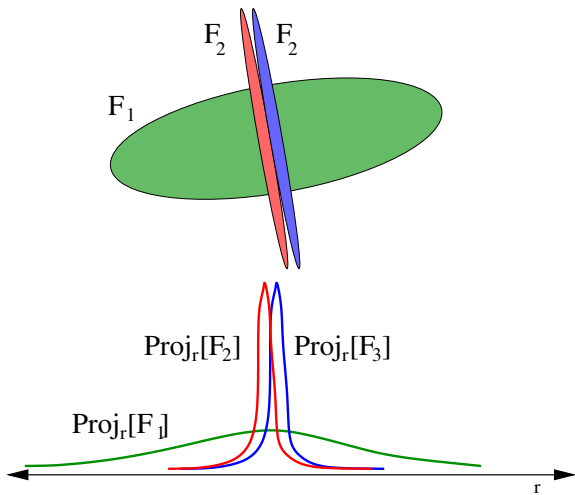


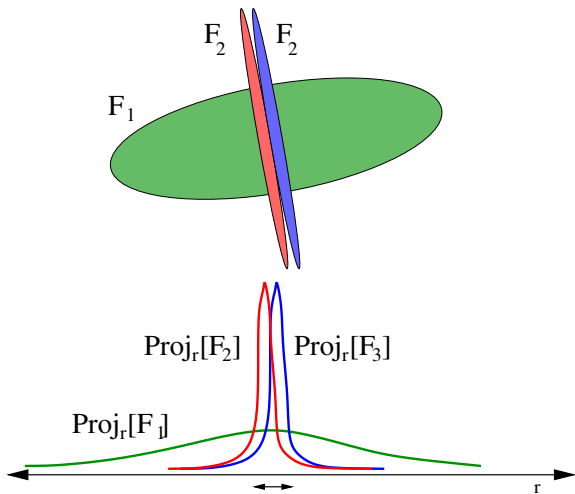
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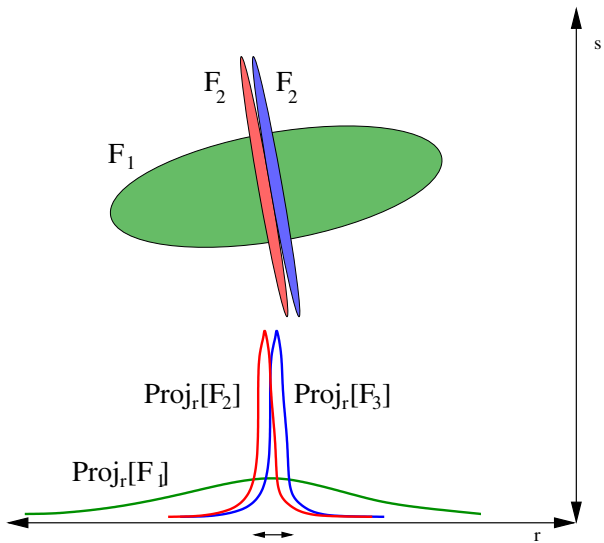


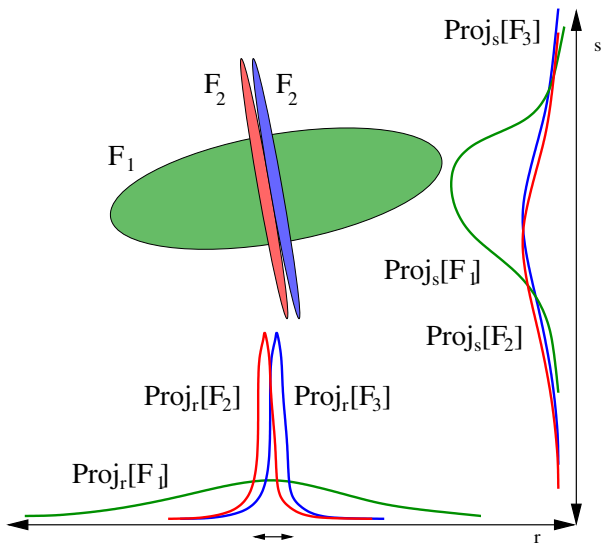


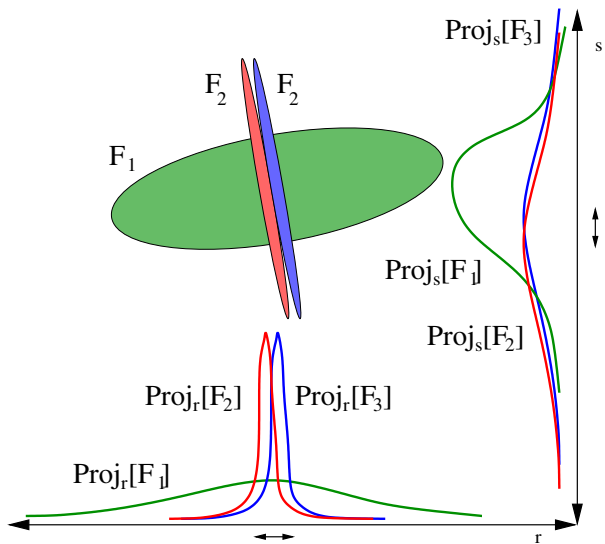












Generalized Isotropic Projection Lemma

Lemma (Generalized Isotropic Projection Lemma)

With probability $\geq 1 - \delta$ over a randomly chosen direction r , for all $i \neq j$,
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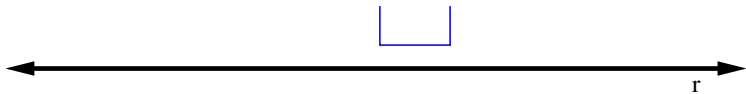
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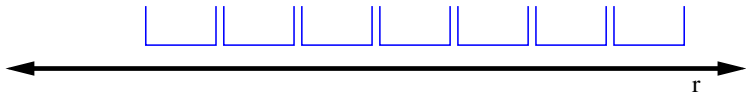
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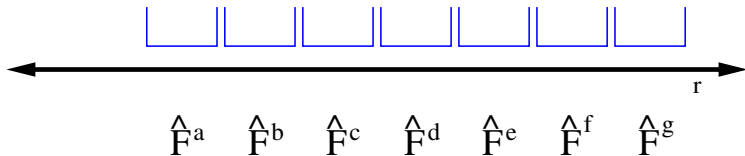
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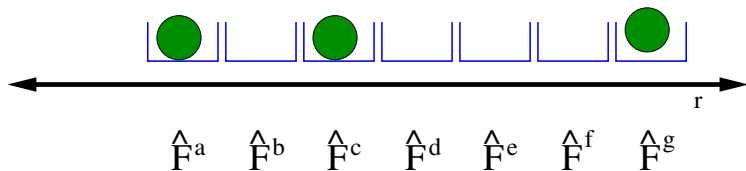
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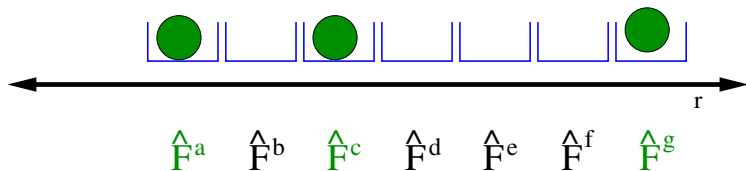
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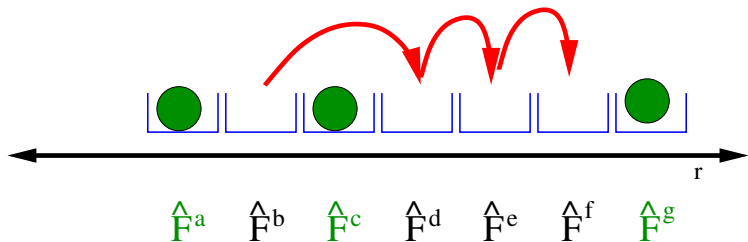
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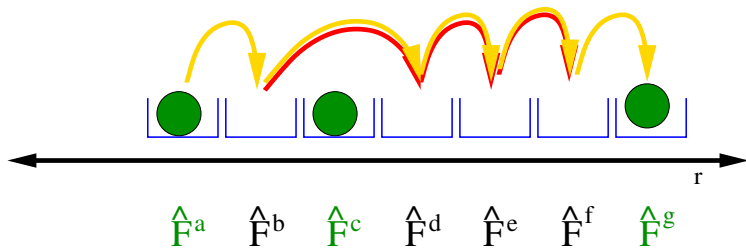
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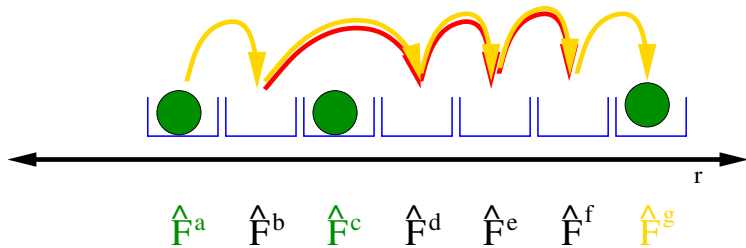
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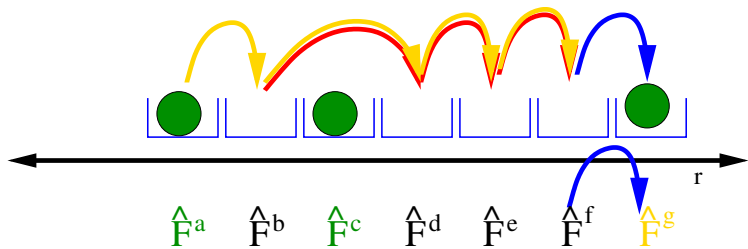
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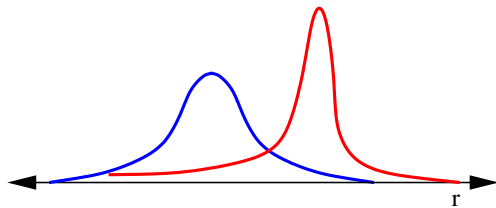
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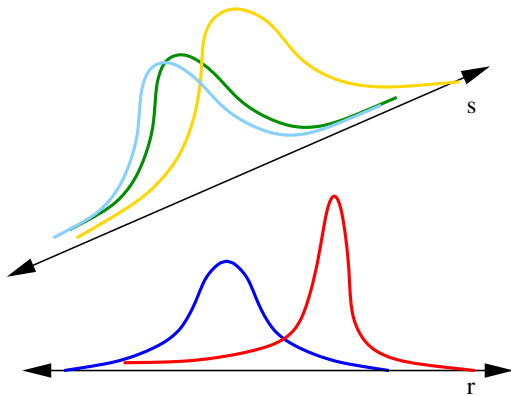
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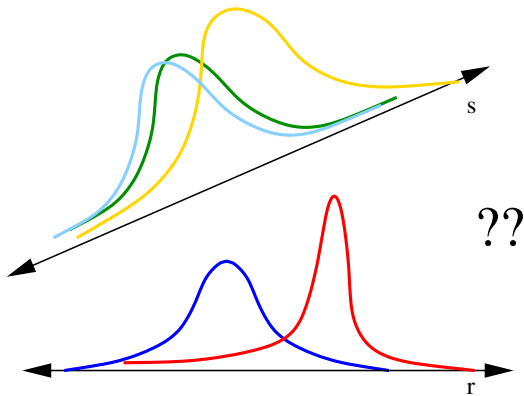
Pairing Lemma, Part 2?



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Thanks!