Lecture 01: Curse of Dimensionality: Problem and Solutions

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30-th of January, 2023



Motivation - Big Data

- Under the 'umbrella' term Big Data, the following is understood to hold:
 - a) Very big number of observations (or data points)
 - b) Very big number of dimensions (or parameters) associated with each data point
- Example for a)
 - The monthly incomes of the residents of Tatarstan
 - Hence, each month we have 3.8 million observations (or data points), which is big.
 - In one year, we will have 45.8 million observations, which is big.
 - BUT NOTE, the dimension is one, since for each person we record only one number. [X1, X2, X155210]
- Example for b)
 - The HD image of the residents of Tatarstan
 - Each image is an observation and each observation is comprised of $1440 \times 1080 = 1,555,200$ pixels, and each pixel represents one dimension. Hence, 1,555,200 dimensions per observation big num.
 - Other examples: text, sound, video, human genome, etc



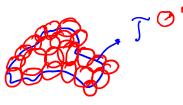
Difficulty - Big Data

- Empirically (i.e., by experience), it is exponentially harder to deal with large number of dimensions than to deal with large number of observations
- Large number of observations is usually not a problem. This has been dealt with tools from classical statistics.
- In fact, the more observations we help, the more we can understanding the statistics (i.e., of what is going on) of the underlying random process.
- But large number of dimensions makes the problem of understanding the statistics very difficult.
- In fact, adding more dimensions to an observation makes the problem of understanding the statistics exponentially more difficult.

Volume of Big Data - Curse of Dimensional

- Example of volume of a cube in high dimensions:
 - The volume of a 2-dimensional cube, where each size is a, is $a \times a = a^2$. For a = 2, the volume is 2^2
 - The volume of a 3-dimensional cube, where each size is a, is $a \times a \times a = a^3$. For a = 2, the volume is 2^3
 - The volume of a d-dimensional cube, where each size is a, is $a \times a \times ... \times a = a^d$. For a = 2, the volume is 2^d .
 - Hence, the volume grows exponentially with the dimension d. This means the for higher dimensions, there is exponentially more space than in lower dimensions.
- This phenomenon is known as the "curse of high-dimensionality" (CD), and is the main problem in DS and ML.
- We have to find methods that can go around the "curse of high-dimensionality", if possible.
- This course is aimed to help you understand how to do that.

• Assume we have an object, described as a set \mathcal{T} , and assume we have N balls or radius r. We would like to completely cover the object with the minimum number of balls. Let us denote this number as $N(\mathcal{T}, r)$. Now how to find $N(\mathcal{T}, r)$ for a given \mathcal{T} and r?

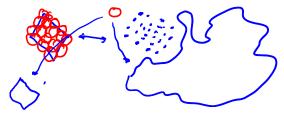


- Def: The covering number of a set $\mathcal{T} \subset \mathbb{R}^d$ and given radius r, is the smallest number of Euclidean balls with radius r that completely cover the set \mathcal{T} .
- The covering number $N(\mathcal{T}, r)$ is a descriptor of the complexity of \mathcal{T} . The less the number is, the easier is to describe \mathcal{T} using only $N(\mathcal{T}, r)$ balls of radius r
- Other meaning: The covering is simply the quantization of \mathcal{T} , whereas the covering number gives us the minimum number of quantized points that describe $N(\mathcal{T}, r)$ with a quantization error r.

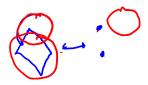


1.553 -> 1 1.56 -> 2

• More accurate quantization for small r, but more points.



ullet More accurate quantization for larger r, but less points.



- The covering number $N(\mathcal{T}, r)$ suffers from the curse of dimensionality: The higher the dimension d of $\mathcal{T} \subset \mathbb{R}^d$ is, exponentially more balls are needed to cover \mathcal{T} , i.e., it is exponentially harder to describe it via balls of fixed radius.
- Fact: If $\mathcal{T} \subset \mathbb{R}^d$ is the unit (radius one) Euclidean ball in dimension d, and we need to cover it by balls of radius r = 1/2, the we would need $N(\mathcal{T}, 1/2) \geq 2^d$ number of balls.
- \circ Note, the above number is exponential in d, hence, CD hits!
- \bullet Proof of the Fact: The volume of a r-radius ball in d dimension is

$$V(d,r) = \frac{\pi^{d/2}}{\Gamma(d/2+1)} r^{d} \qquad \Gamma(n) \approx (h-n) / (h-n) /$$

Hence,
$$\frac{\text{V of big ball}}{\text{V of small ball}} = \frac{V(d,1)}{V(d,1/2)} = \frac{1}{1/2^d} = 2^d$$

On the other hand $V(d,1) \leq N(\mathcal{T}, 1/2)V(d,1/2)$, from where we obtain $N(\mathcal{T}, 1/2) \geq V(d,1/2)/V(d,1/2) = 2^d$.

- Note on the influence of the dimension on the volume of balls:
- Comparing the unit ball with any other ball of radius r < 1, we 厂= 1-2 obtain

$$\frac{\text{V of smaller ball}}{\text{V of unit ball}} = \frac{V(d,r)}{V(d,1)} = \underline{r^d \to 0 \text{ as } d \to \infty}$$

Comparing the unit ball with any other ball of radius r > 1, we obtain

$$\frac{\text{V of larger ball}}{\text{V of unit ball}} = \frac{V(d,r)}{V(d,1)} = \underline{r^d} \to \infty \text{ as } d \to \infty$$
hen the dimension increases, the balls bifurcate into two

- Hence, when the dimension increases, the balls bifurcate into two classes of balls compared to the unit ball
 - One class is balls with r < 1: These balls are almost infinitely smaller than the unit ball
 - Second class is balls with r > 1: These balls are almost infinitely larger than the unit ball



- The above CD happens not just for balls, but for many other objects in high-dimensions. In fact, for almost all high-dimensional objects.
 - This means that it is very likely we to work with high-dimensional data that suffers from the CD, since almost all high-dimensional objects suffer from the CD.
- There are only few high-dimensional objects that do not suffer from the CD. One of these is the polytope.
 - This means that it is very unlikely we to work with high-dimensional data that does not suffers from the CD, since there are few high-dimensional objects that do not suffer from the CD.
- Then how can we avoid CD? We avoid it by not seeking to obtain exactly correct results. Instead, we seek to obtain approximately correct results.

• Numerical integration in dimension d: Let us have a d-dimensional function $g(x_1, x_2, ..., x_d)$. We want to numerically compute the following integral

$$I_d = \int_0^1 \int_0^1 \dots \int_0^1 g(x_1, x_2, \dots, x_d) dx_1 dx_2 \dots dx_d$$

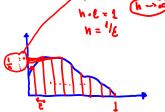
• When d = 1, we have

$$I_1 = \int_0^1 g(x) dx$$

• To approximately compute I_1 , we pick n equally-distant points $\hat{x}_1, \hat{x}_2, ..., \hat{x}_n$, each in D1, with distance ϵ between neighboring points, and compute $1 \sum_{i=1}^{n} f_i(x_i) = 0$

$$\frac{1}{n}\sum_{i=1}^{n}g(\hat{x}_{i})\approx I_{1}$$

- Note that we have used $n = 1/\epsilon$ number of points
- Figure:



• When d=2, we have

$$I_2 = \int_0^1 \int_0^1 g(x_1, x_2) dx_1 dx_2$$

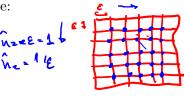
$$I_2 = \int_0^1 \int_0^1 g(x_1, x_2) dx_1 dx_2$$
• To approximately compute I_2 , we pick n equally-distant points

To approximately compute I_2 , we pick n equally-distant points $\hat{x}_1, \hat{x}_1, ..., \hat{x}_n$ in D2, with distance ϵ between neighboring points in each dimension, and perform

$$\frac{1}{n} \sum_{i=1}^{n} g(\hat{x}_i) = \frac{1}{n} \sum_{i=1}^{n} g(\hat{x}_{1i}, \hat{x}_{2i}) \approx I_2$$

- Note that each \hat{x}_i represents a vector of two points given by $\hat{x}_i = [\hat{x}_{1i}, \hat{x}_{2i}]$, where \hat{x}_{1i} is the point from first dimension and \hat{x}_{2i} is the point from second dimension.
- Note that $\epsilon = x_{1i+1} x_{1i} = x_{2i+1} x_{2i}$
- Note that we have used $n = 1/\epsilon^2$ number of points, which can be seen in the next figure.

• Figure:



• When d = d, we have

$$I_d = \int_0^1 \int_0^1 \dots \int_0^1 g(x_1, x_2, \dots, x_d) dx_1 dx_2 \dots dx_d$$
 each vec has a felium but one one of the felium but of the felium but one of the felium but one of the felium but of the feliu

To approximate compute I_d , we pick n equally-distant points $\hat{x}_1, \hat{x}_1, ..., \hat{x}_n$ in $\mathrm{D}d$, with distance ϵ between neighboring points in each dimension, and perform

$$\frac{1}{n} \sum_{i=1}^{n} g(\hat{x}_i) = \frac{1}{n} \sum_{i=1}^{n} g(\hat{x}_{1i}, \hat{x}_{2i}, ..., \hat{x}_{di}) \approx I_d$$

- Note that each $\hat{\boldsymbol{x}}_i$ represents a vector of d points given by $\hat{\boldsymbol{x}}_1 = [\hat{x}_{1i}, \hat{x}_{2i}, ..., \hat{x}_{di}]$, where \hat{x}_{ki} is the point in the k-th dimension of $\hat{\boldsymbol{x}}_i$, for k = 1, 2, ..., d and i = 1, 2, ..., n.
- Note that we have used $n = 1/\epsilon^d$ number of points, and this cannot be even illustrated by a figure.
- If d is large we will be out of memory \rightarrow Uncomputable for large d!

- Now lets try to compute the *d*-dimensional integral using probabilistic tools.
- Instead of picking ϵ -distant $1/\epsilon^d$ points, lets pick n random points $\hat{\boldsymbol{x}}_1, \hat{\boldsymbol{x}}_1, ..., \hat{\boldsymbol{x}}_n$, where each $\hat{\boldsymbol{x}}_i = [\hat{x}_{1i}, \hat{x}_{2i}, ..., \hat{x}_{di}]$ is chosen independently and identically according to the multivariate uniform distribution

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{k=1}^{d} f_{X}(x_k),$$

where

$$f_X(x) = \begin{cases} 1 & \text{if } 0 \le x \le 1\\ 0 & \text{if otherwise} \end{cases}$$

• Then let's compute

$$\frac{1}{n}\sum_{i=1}^{n}g(\hat{x}_i) = \frac{1}{n}\sum_{i=1}^{n}g(\hat{x}_{1i},\hat{x}_{2i},...,\hat{x}_{di})$$

• How close is the above sum to I_d ?

- If we repeat the above process many times, we can consider that $\hat{x}_1, \hat{x}_1, ..., \hat{x}_n$ are n independent and identically distributed (i.i.d.) random vectors.
- Then we can compute the average of the sum as

can compute the average of the sum as
$$E\left[\frac{1}{n}\sum_{i=1}^{n}g(\hat{x}_{i})\right] = \frac{1}{n}\sum_{i=1}^{n}E[g(\hat{x}_{i})] \stackrel{(a)}{=}E[g(\hat{x})],$$

where (a) follows due to the i.i.d. construction of the \hat{x}_i 's. Next,

$$E[g(\hat{\boldsymbol{x}})] = \int_0^1 \int_0^1 \dots \int_0^1 g(x_1, x_2, \dots, x_d) \prod_{k=1}^d f_X(x_k) dx_1 dx_2 \dots dx_d$$

$$\stackrel{(b)}{=} \int_0^1 \int_0^1 \dots \int_0^1 g(x_1, x_2, \dots, x_d) dx_1 dx_2 \dots dx_d = I_d$$

- where (b) follows due to the definition of $f_X(x)$.
- We have obtained that the constructed sum is an unbiased estimator of I_d .

• We have obtained that the average of the constructed sum is equal to I_d . But, what is the error we are making? We can compute the mean squared error (MSE) as

$$E\left[\left(\frac{1}{n}\sum_{i=1}^{n}\widehat{g(\hat{\boldsymbol{x}_i})} - I_d\right)^2\right] = \frac{1}{n^2}E\left[\left(\sum_{i=1}^{n}g(\hat{\boldsymbol{x}_i}) - nI_d\right)^2\right]$$

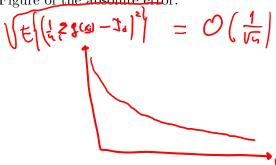
$$= \frac{1}{n^2}VAR\left[\sum_{i=1}^{n}g(\hat{\boldsymbol{x}_i})\right] \stackrel{(a)}{=} \frac{1}{n^2}\sum_{i=1}^{n}VAR\left[g(\hat{\boldsymbol{x}_i})\right] = \frac{1}{n^2}nVAR\left[g(\hat{\boldsymbol{x}})\right]$$

$$= \frac{1}{n}VAR\left[g(\hat{\boldsymbol{x}})\right],$$
where (a) is due to the initial

where (a) is due to the i.i.d.

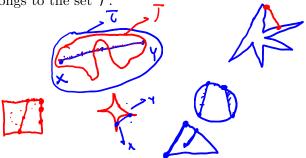
- Hence, the MSE decays with 1/n. This means that the absolute error, defined as $\sqrt{\text{MSE}}$, decays with $1/\sqrt{n}$
- Note, the absolute error (and MSE) is independent from the dimension d! We have avoided the curse of dimensionality!

• Figure of the absolute error:



Def: A set $\mathcal{T} \subset \mathbb{R}^d$ is called a convex set if $\forall x \in \mathcal{T}$ and $\forall y \in \mathcal{T}$, the point $\lambda x + (1 - \lambda)y \in \mathcal{T}$, for any $0 \le \lambda \le 1$.

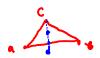
• The above simply means that any point on the line between x and y also belongs to the set \mathcal{T} .



- A way of transforming a non-convex set into a convex set is called taking The Convex Hull
- Def: The convex hull of $\mathcal{T} \subset \mathbb{R}^d$, denoted by conv(f) is the smallest convex set that contains f.
- Note $\mathcal{T} \subset \operatorname{conv}(\overline{\mathbf{f}})$.
- Examples:
 - $\mathcal{T} = \{a, b\}$, then $(\mathcal{T}) = [a, b]$, which denotes the line segment between a



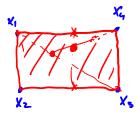
• $\mathcal{T} = \{a, b, c\}$, then





- Fact: (Convex Combination) If $\boldsymbol{x} \in \text{conv}(\mathcal{T})$, then $\boldsymbol{x} = \sum_{i=1}^{m} \lambda_i \boldsymbol{x}_i$, where $\boldsymbol{x}_i \in \mathcal{T}$ and $\lambda_i \geq 0$, $\forall i$, and $\sum_{i=1}^{m} \lambda_i = 1$.
- Caratheodori Thm: $\forall \boldsymbol{x} \in \text{conv}(\mathcal{T})$, where $\mathcal{T} \subset \mathbb{R}^d$, can be expressed as a convex combination of at most d+1 points (read vectors) in \mathcal{T} .
- The above means that any $x \in \text{conv}(\mathcal{T})$ can be described using at most d+1 other vectors in \mathcal{T} , even though the set $\text{conv}(\mathcal{T})$ itself contains infinitely many vectors.
- Hence, we can store infinitely many vectors just by storing at most d+1 other vectors, which is a form of lossless compression.
- Other applications are in optimization: see paper "Fast and Accurate Least-Mean-Squares"

Ex: $\mathcal{T} = \{x_1, x_2, x_3, x_4\}$, where $\forall x_i \in \mathbb{R}^d$. Then $conv(\mathcal{T})$ is rectangle with ∞ points.



- What if we want to describe/store all points in $conv(\mathcal{T})$ with less then d+1 points/vectors, in order to save storage space, i.e., we want to do lossy compression?
- What kind of an error we would make in that compression process?
- In fact, it turns out that we can describe x with an error by choosing m < d, and m is independent of d. Avoided the CD!
- This is described in the following

• Approximate Caratheodori Th (ACT): Let $\mathcal{T} \subset \mathbb{R}^d$, and let $\operatorname{diam}(\mathcal{T}) \leq 1$. Then, $\forall \boldsymbol{x} \in \operatorname{conv}(\mathcal{T})$ and $\forall k \in \mathbb{N}, \exists \boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_k \in \mathcal{T}$ such that



$$\left\| oldsymbol{x} - rac{1}{k} \sum_{i=1}^k oldsymbol{x}_k
ight\|_2 \le rac{1}{\sqrt{2k}}$$

- diam (\mathcal{T}) < 1 means that the length between any two points in \mathcal{T} is at most one. This is just scaling, since we can always divide the points in \mathcal{T} by a scalar such that diam $(\mathcal{T}) < 1$ holds.
- Note the equal weights above, i.e., $\lambda_i = 1/k$, $\forall i$.
- Note $||x||_2 = \sum_{i=1}^d x_i^2$, where x_i is the *i*-th element of x.
- Compression: Hence, instead of storing the infinite number of vectors in conv(\mathcal{T}) using at most d+1 vectors in \mathcal{T} , I can store $\operatorname{conv}(\mathcal{T})$ using $k \ll d$ vectors in \mathcal{T} , and the squired error that I would make is at most $1/\sqrt{2k}$.

$$\mathbb{E}((x-\hat{x})^2) = \mathbb{E}(x^2 - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(\hat{x}^2) - 2\mathbb{E}(x) \cdot \mathbb{E}(\hat{x} - 2x\hat{x} + \hat{x}^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2) + \mathbb{E}(x^2) + \mathbb{E}(x^2) = \mathbb{E}(x^2$$

- How can we achieve the (ACT)? Using probability, and this is how
 First, another definition of VAR[X]:

$$VAR[X] = \frac{1}{2}E[(X - \hat{X})^2],$$

where \hat{X} is i.i.d. as X, and X is one dimensional. Prove this at home!

Similarly, for random vectors: If $X \in \mathbb{R}^d$, then

$$VAR[\mathbf{X}] = E\left[||\mathbf{X} - E[\mathbf{X}]||_2^2\right] = \frac{1}{2}E\left[||\mathbf{X} - \mathbf{L}\hat{\mathbf{X}}||_2^2\right], \quad (2)$$

where \hat{X} is i.i.d. as X. Again, prove at home!

• Proof of ACT: Fix $x \in \text{conv}(\mathcal{T})$. Then, we know that

$$oldsymbol{x} = \sum_{i=1}^{d+1} \lambda_i oldsymbol{z}_i,$$

where $z_i \in \mathcal{T}$, $\lambda_i \geq 0$ and $\sum_{i=1}^{d+1} \lambda_i = 1$.

We now interpret λ_i 's as probabilities and the above sum as expectation.

Let Z be a discrete random vector with PMF $\Pr\{Z = z_i\} = \lambda_i$. Then,

$$\boldsymbol{x} = E[\boldsymbol{Z}] = \sum_{i=1}^{d+1} \lambda_i \boldsymbol{z}_i \tag{3}$$

Now let us take k RVs that are i.i.d. as \mathbf{Z} , given by $\mathbf{Z}_1, \mathbf{Z}_2, ..., \mathbf{Z}_k$.

Then, we know that

we know that
$$E\left[\left\|\frac{1}{k}\sum_{i=1}^{k} \mathbf{Z}_{i} - E[\mathbf{Z}]\right\|_{2}^{2}\right] \stackrel{(a)}{=} E\left[\left\|\frac{1}{k}\sum_{i=1}^{k} \mathbf{Z}_{i} - \mathbf{x}\right\|_{2}^{2}\right]$$

$$= E\left[\left\|\frac{1}{k}\sum_{i=1}^{k} (\mathbf{Z}_{i} - \mathbf{x})\right\|_{2}^{2}\right] \stackrel{(a)}{=} \frac{1}{k^{2}} E\left[\left\|\sum_{i=1}^{k} (\mathbf{Z}_{i} - E[\mathbf{Z}_{i}])\right\|_{2}^{2}\right]$$

$$= \frac{1}{k^{2}} VAR\left[\sum_{i=1}^{k} \mathbf{Z}_{i}\right] = \frac{1}{k^{2}} \sum_{i=1}^{k} VAR[\mathbf{Z}_{i}] = \frac{1}{k} VAR[\mathbf{Z}]$$

$$\stackrel{(b)}{=} \frac{1}{2k} E\left[\left\|\mathbf{Z} - \mathbf{Z}_{1}\right\|\right]_{2}^{2} \stackrel{(c)}{\leq} \frac{1}{2k} \operatorname{diam}(\mathcal{T})^{2} \stackrel{(d)}{\leq} \frac{1}{2k},$$

where (a) is due to (3), (b) is due to (2), and c is due to the fact that the diffrence between any two points cannot be larger than $\operatorname{diam}(\mathcal{T})$, and (d) is due to $\operatorname{diam}(\mathcal{T}) \leq 1$

Now, since

$$E\left[\left\|\frac{1}{k}\sum_{i=1}^{k} \mathbf{Z}_{i} - \mathbf{x}\right\|_{2}^{2}\right] \leq \frac{1}{2k} \tag{4}$$

then $\exists z_1, z_2, ..., z_k \in \mathcal{T}$ (read there exist k realizations of \mathbf{Z}) such that

$$\left\| \frac{1}{k} \sum_{i=1}^{k} \boldsymbol{z}_i - \boldsymbol{x} \right\|_2^2 \le \frac{1}{2k} \tag{5}$$

from which

$$\left\| x - \frac{1}{k} \sum_{i=1}^{k} z_i \right\|_{\mathcal{L}} \le \frac{1}{\sqrt{2k}} \tag{6}$$

Example of ACT

- We age given n images represented as vectors $\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n$, where $\boldsymbol{x}_i \in \mathbb{R}^d$, $\forall i$. Let x_{ji} be the j-th element of \boldsymbol{x}_i , where x_{ji} represents the j-th pixel of the image \boldsymbol{x}_i .
- We would like to create a new image x (of some desired shapes), by mixing some or all of the given images $x_1, x_2, ..., x_n$, i.e., by convex combination of the given images. Mathematically,

$$oldsymbol{x} = \sum_{i=1}^n \lambda_i oldsymbol{x}_i,$$

where $\lambda_i \geq 0$ and $\sum_{i=1}^n \lambda_i = 1$.

• We must assume that the desired image x can indeed the formed as a convex combination of $x_1, x_2, ..., x_n$. More precisely, x belongs to the convex hull created from $x_1, x_2, ..., x_n$, i.e., $x \in \text{conv}(\{x_1, x_2, ..., x_n\})$. Otherwise, the desired image cannot be created.



Example of ACT

- What the Caratheodori Theorem tells us, is that we need to mix at most d+1 images to create the desire image \boldsymbol{x} . If the image is HD, thereby contains, $d=1440\times1080=1,555,200$ pixels, we need to mix 1,555,200+1 images to obtain the desire image.
- What the Approximate Caratheodori Theorem tells us, is that we need to mix at most k images to create the desire image \boldsymbol{x} . If we mix k=100 images, then the absolute mean error between the original and the approximated image will be
- 11.100
- 1/(2 * 10) = 0.06 = 6%, which might be a very close approximation that the eye cannot notice.
 - Note: The Approximate Caratheodori Theorem shows only existence of the points that make the approximations, but do not shows us how to obtain these points, other by brute-force search. Hence, the search for such an algorithm is ongoing.