grain size analysis

grains
particles in matrix

processes - theoretical models:
fluvial transport
wind transport
growth
winnowing
sedimentation
flotation
sediment mixing
...

grains
crystals in solid

processes - theoretical models:
dynamic recrystallization
magma cooling
annealing - grain growth
metamorphic reaction
...

grains
voids

processes - theoretical models:
ice (cream)
bubble formation
bubble growth
volcanoes
pore formation
pore deformation
...
We will describe grain size - and grain size distributions - in terms of a single length parameter. In other words we will think about size as a scalar and we will not consider any influence of shape and preferred orientations. To describe size quantitatively we will use the concept of equivalent radius or equivalent diameter:

- the equivalent radius ($r_e$) of a 2-D outline is the radius ($r$) of the circle that contains the same area as the shape in question.
- the equivalent diameter ($d_e$) of a 2-D outline is the diameter ($d$) of the circle that contains the same area as the shape in question.
- the equivalent radius ($R_e$) of a 3-D particle is the radius ($R$) of the sphere that contains the same volume as the particle in question.
- the equivalent diameter ($D_e$) of a 3-D particle is the diameter ($D$) of the sphere that contains the same volume as the particle in question.

We will represent size distributions as continuous density functions or discrete histograms $h(r)$ or $h(d)$.

Usually, what we obtain from measurements are histograms and what we fit to the data are continuous functions.

Many naturally occurring size distributions can be approximated by relatively simple mathematical functions, most notably the Gaussian normal, but there are just as many which defy such approximations.

In cases where we find a suitable function that describes the measured distribution, we can recalculate the distribution from the equation and the coefficients. This is more efficient than listing all the size classes and their frequencies. (It is more efficient, but it may be misleading…).

We will distinguish 2-D and 3-D size distributions. By this we mean distributions that describe populations of 2-D and 3-D objects (the distributions as such do not really have any dimensions at all…).

As an example we will look at size distributions of 3-D objects (or particles) such as sand grains, tomatoes, pebbles, cabbage heads, …

The monodisperse distribution describes a population where all particles are of the same size.
- $h(R) = 1.00$ if $R = R_K$
- $h(R) = 0.00$ if $R \neq R_K$

The uniform distribution characterises a population where all sizes are equally probable.
- $h(R) = \text{constant}$
  (this is sometimes called the random distribution)
The normal distribution describes a population with one preferred size $\mu$ and a certain spread about it

$$h(R) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(R-\mu)^2}{\sigma^2}\right)$$

where $\mu = \text{mean}$ and $\sigma = \text{standard deviation}$

The normal distribution is also called the Gaussian or Gauss normal distribution.

The normal distribution is completely defined by $\mu$ and $\sigma$, i.e., there is exactly one Gaussian normal distribution for a given pair of $\mu$ and $\sigma$. Large $\sigma$ - values indicate large dispersions (spread about the mean), the corresponding populations are poorly sorted. In the limit, if $\sigma \to \infty$, the normal distribution is equal to the uniform distribution, if $\sigma \to 0$, the monodisperse distribution is attained.

There are, however, many other types of distributions which are realized in nature - for some of them, reasonable mathematical descriptions can be found; others cannot be adequately described without using a large number of coefficients or parameters.

We will characterise such distributions in rather more general terms as

- symmetric or asymmetric
- unimodal or bimodal or polymodal

Even though the statistical parameters (mean, variance, skewness and kurtosis) of these distributions can be derived easily, the true nature of the distribution cannot be reconstructed from them (since there is an infinite number of different distributions which yield the same mean, variance, etc.). In these cases, the distributions are best given as full listings of frequencies for all size classes.

Size distributions are plotted as histograms or density functions.

Choosing a linear $x$ - axis implies regular sampling intervals $\Delta x$, i.e., a constant width along the linear length axis.

Choosing a logarithmic $x$ - axis implies regular sampling intervals in logarithm space $\ln(x)$, i.e., a constant width along the logarithmic length axis.

Important: When logarithmic histograms are converted to linear, the bin size is not constant anymore, i.e., the classes are not regularly spaced and the function is not a density function anymore.
For sieving measurements, the so-called $\Phi$-values are used:

$$\Phi = -\log_2(d)$$

where $d$ = diameter measured in mm

$$\log_2(x) = \frac{\log_{10}(x)}{\log_{10}(2)} \cdot \log_{10}(x)$$

$$\log_2(x) = 3.32 \cdot \log_{10}(x)$$

When $\Phi$-value histograms are converted to linear, the bin size is not constant anymore, i.e., the classes are not regularly spaced.

For the y-axis of a histogram there are a number of options. In the context of image analysis or point counting we generally use numerical densities.

- counts
- relative counts or percentage

Another option for histograms are the so-called ogives, where the measured (sieved) data is plotted against cumulative frequencies $\Sigma%$.

This representation is used in sedimentological studies in the context of sieving analyses of loose sediments.

Other plots with cumulative frequencies and natural logarithms are used, where $\Sigma h(L_i) = \text{cumulative frequency}$

$$L_i = \text{largest horizontal diameter}$$

Population density

$$n = \frac{dN}{dL}$$

$$N_i = \Sigma h(L_i) \cdot \frac{3}{2}$$

$3/2 = \text{sterological correction}$

Such representations are favoured by magmatic petrologists in order to study crystal size distributions (CSD) of cooling magma.
choice of coordinates

In image analysis, grain size is often measured as sectional area. In this case, the y-axis is number density but the linear x-axis is area (mm$^2$) (top). It is obvious that simply transforming the x-axis will not transform $h(a)$ into $h(r_e)$. Instead the areas have to be converted to radii and the data is plotted as length (mm) on the linear x-axis (bottom).

$h(a)$
The number of sections with an area ($a$) of a given size (mm$^2$) is described by the numerical density histogram $h(a)$.

$h(r_e)$
The number of sections with an equivalent radius ($r_e$) of a given length (mm) is described by the numerical density histogram $h(r_e)$.

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**3-D to 2-D**

spheres to circles

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which grains?

In the following we will assume a very simple situation. We will address the problem of diluted particles on a matrix.

This is a good enough approximation to many sedimentological situations but does not seem to be appropriate - at first - for crystalline aggregates.

We will further assume isotropy of shape and spatial distribution. In short, the particles are spheres (of various size) which are widely spaced such that the occurrence of one at any given site does not influence the occurrence of another one.

Strictly speaking, this is not true because in our physical world it is impossible for one grain to exist at the same locality where another one is already present. For diluted fabrics, it is "approximately true".
model for random sectioning process

In order to calculate the distribution of sectional circles of a population of spheres on a 2-D plane, we create the following conceptual model:

- A population of spheres is randomly distributed in space. The average distance between the centers of the spheres is much larger than their average diameter (diluted fabric).
- A sectioning plane is placed at random. The probability of intersecting a sphere depends on the size of the sphere. The size of the sectional circle depends on where - along the diameter - the sphere is intersected.

1. What is the size distribution $h(r)$ of sectional circles from one sphere $R$?
2. What is the size distribution $h(R)$ of sectional circles from a population of spheres $h(R)$?

$h(r)$ for one sphere $R$

We will first consider the problem of sectioning a single sphere.

$R$ = radius of sphere
$r$ = radius of sectional circle
$d$ = distance of center of sphere from sectioning plane

The radius of the sectional circle is given by:

$$r = \sqrt{R^2 - d^2}$$

If we section the sphere at regular intervals $\Delta d$, we do not obtain a uniform distribution of sectional circles, we obtain rather more big sections than small ones.

$h(r)$ for one sphere $R$

In order to calculate the distribution of the radii of the sectional circles, we have to "invert" the question. We have to ask where - along the diameter $2R$ - the sphere must be cut in order to produce a section of a given size. We need to derive the intercept - along $2R$ - which produces sections in a given constant interval $\Delta r$ of the radius of the sectional circles.

For given $\Delta r$, find $\Delta d$. The proportion of $\Delta d$ relative to $R$ is the probability of obtaining sections with a radius in a given interval $\Delta r$.

$$\frac{\Delta d}{R} = \text{probability for radius in interval} \{r, (r+\Delta r)\}.$$
2-D sections from 3-D particles

The derivation of size distributions \( h(r) \) from size distributions \( h(R) \) is straightforward.

For description, see GrainSize.pdf.

Use program CalSecDis and distribution files

(http://www.unibas.ch/arth/micro -> software)

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### monodisperse \( h(R) \)

This distribution is also called the Delta function

\[
\begin{align*}
\text{h}(r) & \quad \text{h}(R) \\
\end{align*}
\]

### uniform \( h(R) \)

All sizes are equally probable

\[
\begin{align*}
\text{h}(r) & \quad \text{h}(R) \\
\end{align*}
\]

### normal \( h(R) \)

This distribution is also called the Gaussian normal distribution. In this example, the standard deviation is approximately 1/6 of the visible range.

\[
\begin{align*}
\text{h}(r) & \quad \text{h}(R) \\
\end{align*}
\]
For the derivation of size distributions \( h(R) \) from size distributions \( h(r) \) the program StripStar is used. For description, see GrainSize.pdf.

Use program StripStar and optional input files:

(http://www.unibas.ch/earth/micro >> software)
inverting the problem: 3-D from 2-D

reference distribution = uniform \( h(r) \)

\[
\sum h(r) \text{ for } h(R_1) \ldots h(R_{\text{max}})
\]

StripStar program

First step:
from the \( h(r) \) of the uniform \( h(R) \) the contribution to \( h(r) \) of \( R_k \) (where \( R_k = R_{\text{max}} = R_{10} \)) is subtracted,
leaving a "stripped" distribution \( h(r) \)
a unit amount is assigned to \( h(R_k) \), the maximum class of spheres.

StripStar program

Second step:
from the "stripped" \( h(r) \) of the uniform \( h(R) \) the contribution to \( h(r) \) of \( R_{k-1} \) (where \( R_{k-1} = R_9 \)) is subtracted.
a proportional amount is assigned to \( h(R_{k-1}) \)

StripStar program

3rd step:
from the "stripped" \( h(r) \) of the uniform \( h(R) \) the contribution to \( h(r) \) of \( R_{k-n+1} \) (where \( R_{k-n+1} = R_8 \)) is subtracted.
a proportional amount is assigned to \( h(R_{k-n+1}) \)
4th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted.

A proportional amount is assigned to $h(R_{k-n+1})$

5th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted.

A proportional amount is assigned to $h(R_{k-n+1})$

6th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted.

A proportional amount is assigned to $h(R_{k-n+1})$

7th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted.

A proportional amount is assigned to $h(R_{k-n+1})$
8th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted. A proportional amount is assigned to $h(R_{k-n+1})$

9th step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted. A proportional amount is assigned to $h(R_{k-n+1})$

Last step: from the "stripped" $h(r)$ of the uniform $h(R)$ the contribution to $h(r)$ of $R_{k-n+1}$ (where $R_{k-n+1} = R_k$) is subtracted. A proportional amount is assigned to $h(R_1)$

**Examples:**

- **Monodisperse $h(R)$**
examples

uniform h(R)

h(r)  \rightarrow  h(R)

examples

normal h(R)

h(r)  \rightarrow  h(R)

2D to 3D - circles to spheres

sample size and class width

All frequencies of the starting h(r) are now accounted for.

Convert histogram h(R) to V(R).

If negative frequencies occur (antispheres):

- increase sample size
- increase class width

 StripStar

“Choice of grain size”

- area \rightarrow equivalent radius / diameter
- perimeter
- long axis
- short axis
examples

segmentation I (POP)

From polished section...

...prepare monochrome image (1350·900)
(green channel of RGB picture)
adjust contrast

segmentation I (POP)

Segmentation by Point Operation (POP)

ImageXM-Analyze menu
options: area, perimeter, long axis, short axis, angle
Evaluate particles

Kaleidograph:
calculate equivalent radius or diameter
\[ r = \sqrt{\frac{\text{area} + \text{perimeter}}{\pi}} \]

Kaleidograph: scale lengths and areas
**StripStar**

**Input data:**

Kaleidagraph:
bin data: 10 bins, interval: 4 units
histogram h(r)

Use StripStar (see GrainSize.pdf)

Kaleidagraph view output file (result file):
h(R)
V(R)
h*(R)
V*(R)

**Example:**
oolithic limestone

**StripStar**

**CALCULATED SPHERES**

h(r) = INPUT
numerical density histogram of equivalent radii of 2-D sections (circles), n = 268 (small sample !)

h(R) = OUTPUT
numerical density histogram of equivalent radii of 3-D particles (spheres)

V(R) = OUTPUT
volume density histogram of equivalent radii of 3-D particles (spheres)

**Example:**
oolithic limestone

**StripStar**

**CALCULATED ANTI-/ SPHERES**

h(r) = INPUT
input histogram, n = 268 (small sample !)

h*(R) = OUTPUT
including antispHERES

V*(R) = OUTPUT
including antispHERES

< 1 vol % antispHERES => analysis OK

**Example:**
oolithic limestone

**StripStar**

h(r) = INPUT
numerical density histogram of equivalent radii of 2-D sections (circles), n = 1393

h(R) = OUTPUT
numerical density histogram of equivalent radii of 3-D particles (spheres)

V(R) = V*(R) = OUTPUT
volume density histogram of equivalent radii of 3-D particles (spheres) (0% antispHERES)
StripStar

\[ h(a) = \text{INPUT} \quad (a = \text{long diameter}) \]
numerical density histogram of equivalent radii of 2-D sections (circles), \( n = 1393 \)

\[ h(R) = \text{OUTPUT} \]
numerical density histogram of equivalent radii of 3-D particles (spheres)

\[ V(R) = V^*(R) = \text{OUTPUT} \]
volume density histogram of equivalent radii of 3-D particles (spheres) (0% antisphere)

example:oolithic limestone
axial compression experiment, Black Hills Quartzite
dislocation creep regime 3 dynamic recrystallization

4 input images:
• A: no recrystallization
• B: beginning recrystallization
• C: increasing recrystallization
• D: completely recrystallized

starting grain size: average diameter \( \approx 100 \mu m \)

problem: quantify evolution of 3-D grain size distribution

Use NIH Image & Lazy grain boundaries (Heilbrunner, 2000)
Input images: misorientation images (CIP: computer-integrated polarization microscopy)
Stack of misE, misH, misN

segmentation III (NOP, automatic)
edge detection \( O \) (Sobel filter, gradient image)

adaptive thresholding \( G \) (level = mean of histogram of gradient image)
segregation III (NOP, automatic)

- thinning T
- skeletonizing I
- pruning I

remove rim 5
fill
→ invert Y and save as area

example: recrystallized quartz

ScriptStar

$h(r) = \text{INPUT}$

A. few porphyroclasts < 20% of total count
B. decreasing size and number of porphyroclasts
C. increasing number of recrystallized grains
D. % porphyroclasts % recrystallized ?

example: recrystallized quartz

$V(R) = \text{OUTPUT}$

A. > 95 vol% porphyroclasts
   ~ 5 vol% recrystallized grains
B. ~ 90 vol% porphyroclasts
   ~ 10 vol% recrystallized grains
C. ~ 50 vol% porphyroclasts
   ~ 50 vol% recrystallized grains
D. ~ 15 vol% porphyroclasts
   > 85 vol% recrystallized grains

alternatives