# Data fitting stochastic models

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- Find a good or even best distribution from that family.
- When does a distribution explain data well?

# The Old Faithful data set

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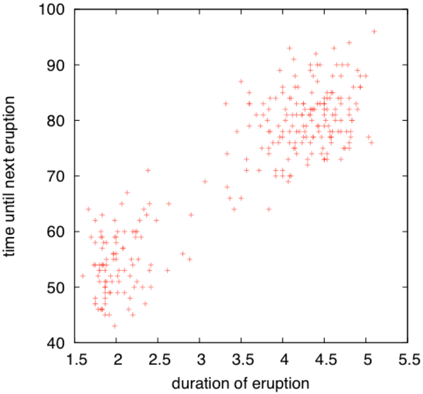

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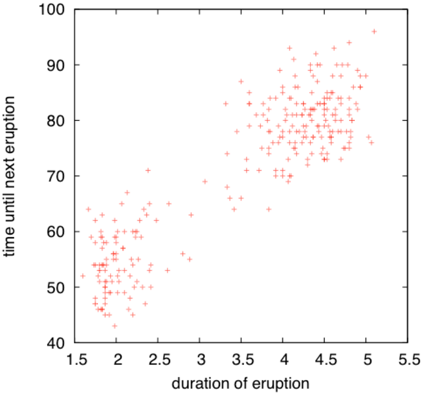


Is there a distribution that explains the apparent dependency between duration and time until next eruption?

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## Families of continuous distributions

- $d \in \mathbb{N}, S \subseteq \mathbb{R}^s$ for some $s \in \mathbb{N}, |S| = \infty$
- for each $\Theta \in S$ a density function $p(\cdot|\Theta) : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, i.e.

$$\int_{\mathbb{R}^d} p(x|\Theta)\mathrm{d}x = 1.$$

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## Example - univariate Gaussian distributions

- $d = 1, S = \mathbb{R} \times \mathbb{R}_{>0}, \Theta = (\mu, \sigma)$
- $p(\cdot|\Theta) = p(\cdot|\mu, \sigma) = \mathcal{N}(\cdot|\mu, \sigma^2)$

## Definition 6.1

*Let* $X \subset \mathbb{R}^d, |X| < \infty$ *and* $\{p(\cdot|\Theta)\}_{\Theta \in S}$ *a family of density functions.*

1. $p(X|\Theta) := \prod_{y \in X} p(y|\Theta)$ *is called the likelihood of* $X$ *with respect to* $p(\cdot|\Theta)$ *or simply with respect to* $\Theta$.
2. $\mathcal{L}_X(\Theta) = -\ln(p(X|\Theta)) = -\sum_{y \in X} \ln(p(y|\Theta)$ *called negative log-likelihood of* $X$ *with respect to* $\Theta$.

## Problem 6.2 (Maximum likelihood estimation)

*Given a family* $\{p(\cdot|\Theta\}_{\Theta \in S}$ *of distributions on* $\mathbb{R}^d$ *and a finite set* $X \subset \mathbb{R}^d$, *find* $\Theta_0 \in S$ *that minimizes the negative log-likelihood* $\mathcal{L}_X(\Theta)$.

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**Remarks**

- Depending on the definition of $S$ the maximum likelihood estimation problem is not well defined.

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**Remarks**

- Depending on the definition of $S$ the maximum likelihood estimation problem is not well defined.
- In other cases, the parameters $\Theta$ that have the minimal negative log-likelihood are not very useful.
- In this case, the goal is to find "useful" or "relevant" parameters $\Theta$ that model the point set $X$.

# Log-likelihood estimation for spherical Gaussians

## Theorem 6.3

*Let* $S = \mathbb{R} \times \mathbb{R}_{>0}$ *and* $p(\cdot|\mu,\sigma) = \mathcal{N}(\cdot|\mu,\sigma^2)$ *for all* $(\mu,\sigma) \in S$. *For a finite point set* $X \subset \mathbb{R}, |X| \geq 2$,

1. *for fixed* $\mu$ *the value for* $\sigma^2$ *minimizing* $\mathcal{L}_X(\mu,\sigma)$ *is given by*

$$\sigma^2 = \frac{1}{|X|} \sum_{y \in X} (y-\mu)^2,$$

2. *the parameters* $\Theta = (\mu,\sigma)$ *minimizing* $\mathcal{L}_X(\mu,\sigma)$ *are given by*

$$\mu = \frac{1}{|X|} \sum_{y \in X} y \quad \text{and} \quad \sigma^2 = \frac{1}{|X|} \sum_{y \in X} (y-\mu)^2.$$

*Consequently, given* $X$ *the optimal values for* $\mu$ *and* $\sigma$ *can be computed in time* $\mathcal{O}(|X|)$.

# Multivariate Gaussians

## Spherical Gaussian distributions

- $d$ arbitrary, fixed, $S = \mathbb{R}^d \times \mathbb{R}_{>0}, \Theta = (\mu, \sigma)$
- $\mathcal{N}(\cdot|\mu, \sigma^2) : \mathbb{R}^d \to \mathbb{R}_{>0}$

$$x \mapsto \frac{1}{(2\pi\sigma^2)^{d/2}} \cdot \exp\left(-\frac{\|x-\mu\|^2}{2\sigma^2}\right)$$

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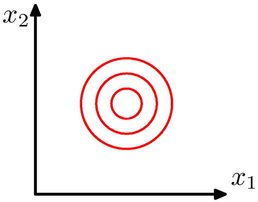
Contours of constant probability density for spherical Gaussians




(c)

## Axis-aligned Gaussian distributions

$d$ arbitrary, fixed, $S \subset \mathbb{R}^d \times \mathbb{R}^d_{>0}, \Theta = (\mu, \sigma_1, \ldots, \sigma_d)$

$$\mathcal{N}(\cdot|\Theta) : \mathbb{R}^d \to \mathbb{R}_{>0}$$
$$x \mapsto \frac{1}{(2\pi)^{d/2}(\prod \sigma_i^2)^{1/2}} \cdot \exp\left(-\sum \frac{(x_i - \mu_i)^2}{2\sigma_i^2}\right)$$

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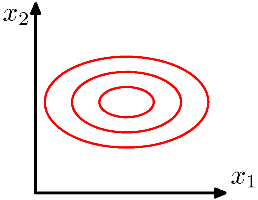
Contours of constant probability density for axis-aligned Gaussians




(b)

## (General) Gaussian distributions

$d$ arbitrary, fixed, $S \subset \mathbb{R}^d \times \mathbb{R}^{d \times d}, \Theta = (\mu, \Sigma), \Sigma$ positive definite

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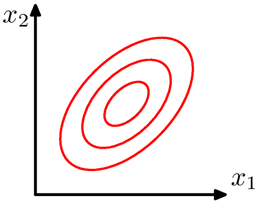
Contours of constant probability density for general Gaussians

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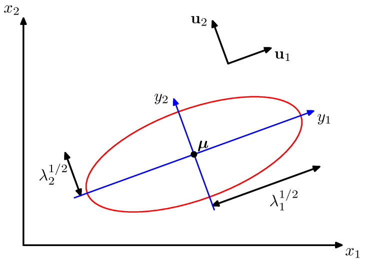
Contour in terms of eigenvalues and eigenvectors of $\Sigma$



# Log-likelihood estimation for spherical multivariate Gaussi

## Theorem 6.4

*Let* $S = \mathbb{R}^d \times \mathbb{R}_{>0}$ *and* $p(\cdot|\mu,\sigma) = \mathcal{N}(\cdot|\mu,\sigma^2)$ *for all* $(\mu,\sigma) \in S$. *For a finite point set* $X \subset \mathbb{R}^d, |X| \geq 2$,

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*Consequently, given* $X$ *the optimal values for* $\mu$ *and* $\sigma$ *can be computed in time* $\mathcal{O}(|X|)$.

## Log-likelihood estimation for multivariate Gaussians

### Theorem 6.5

*Let* $d \in \mathbb{N}, S \subset \mathbb{R}^d \times \mathbb{R}_{d\times d}$, $p(\cdot|\Theta) = \mathcal{N}(\cdot|\Theta), \Theta = (\mu, \Sigma)$, $\Sigma \in \mathbb{R}^{d\times d}$ *positive definite. For a finite point set* $X \subset \mathbb{R}^d, |X| \geq 2$,

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$$\Sigma = \frac{1}{|X|} \sum_{y\in X} (y-\mu)\cdot(y-\mu)^T,$$

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# Mixtures of Gaussians

## Gaussian mixture distributions

- $d, K$ arbitrary, fixed, $\Theta = (\Theta_1, \ldots, \Theta_K, \pi), \Theta_k$ models for $d$-variate Gaussian distributions, $\pi \in \mathbb{R}^k_{\geq 0}, \|\pi\|_1 = 1$
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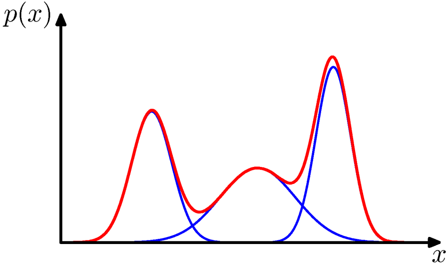
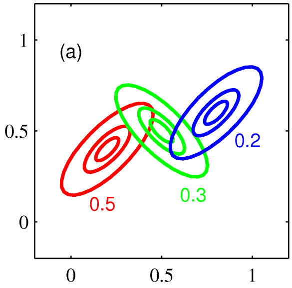
Mixture of three univariate Gaussian distributions



# Mixtures of Gaussians

Contours of constant probability densities for three Gaussians



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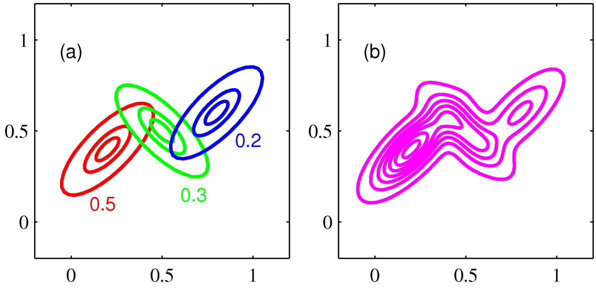
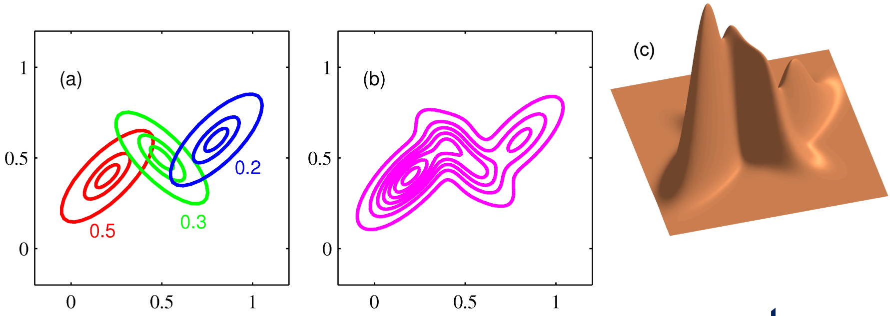


# Mixtures of Gaussians

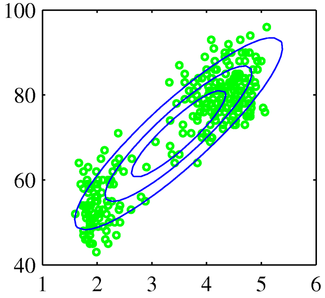
Contours of constant probability densities for three Gaussians

Contours of constant probability densities for mixture of three Gaussians

Surface plot for mixture of three Gaussians

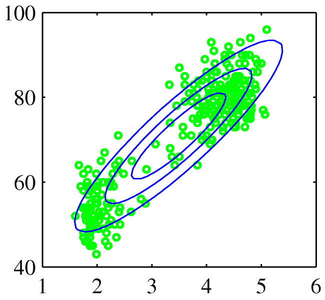


Explaining Old Faithful with a single multivariate Gaussian

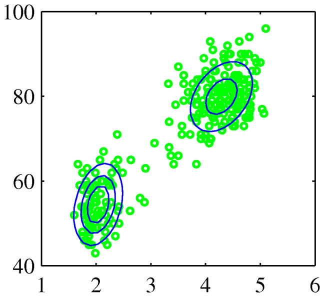


# Old Faithful and mixtures of Gaussians

Explaining Old Faithful with a single multivariate Gaussian




Explaining Old Faithful with a mixture of two multivariate Gaussians

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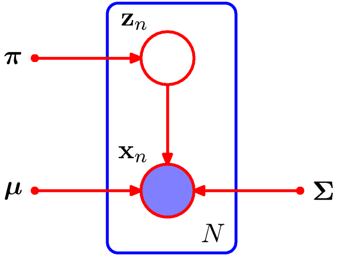
# Graphical representation of Gaussian mixtures




To generate a point distributed according to a mixture of Gaussians:

1. choose an index $k$ according to the distribution $\pi = (\pi_1, \ldots, \pi_K)$
2. choose a point $x$ according to the distribution $\mathcal{N}(\cdot|\Theta_k)$.

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# Likelihood for mixtures of Gaussians

## Gaussian mixture distributions

- $d, K$ arbitrary, fixed, $\Theta = (\Theta_1, \ldots, \Theta_K, \pi), \Theta_k$ models for $d$-variate Gaussian distributions, $\pi \in \mathbb{R}^k_{\geq 0}, \|\pi\|_1 = 1$
- $x \mapsto \sum_k \pi_k \mathcal{N}(x|\Theta_k)$

## Likelihoods

$X \subset \mathbb{R}^d, |X| = N, X = \{x_1, \ldots, x_N\}$

- $p(X|\Theta) = \prod_{n=1}^N p(x_n|\Theta) = \prod_{n=1}^N \left(\sum_{k=1}^K \pi_k \mathcal{N}(x_n|\Theta_k)\right)$
- $\mathcal{L}_X(\Theta) = -\ln(p(X|\Theta)) = -\sum_{n=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\Theta_k)\right)$

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- $x \mapsto \sum_k \pi_k \mathcal{N}(x|\Theta_k)$

## Likelihoods

$X \subset \mathbb{R}^d, |X| = N, X = \{x_1, \ldots, x_N\}$. Set $\mu_1 = x_1, \pi_1 \neq 0$. Then

$$\lim_{\sigma_1 \to 0} \mathcal{L}_X(\Theta) = -\infty,$$

i.e. negative log-likelihood not well-defined.

# Optimality conditions for $d = 1$

No closed formula for

$$\text{argmin}_{\Theta}\mathcal{L}_X(\theta) = \text{argmin}_{\Theta} - \sum_{n=1}^{N} \ln\left(\sum_{k=1}^{K} \pi_k \mathcal{N}(x_n|\Theta_k)\right)$$

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Taking derivatives (with Lagrange multipliers) yields

$$\mu_k = \frac{1}{R_k}\sum_{n=1}^{N} \gamma_{nk} x_n, k = 1, \ldots, K, \quad (1)$$

$$\sigma_k^2 = \frac{1}{R_k}\sum_{n=1}^{N} \gamma_{nk}(x_n - \mu_k)^2, k = 1, \ldots, K, \quad (2)$$

$$\pi_k = \frac{R_k}{N}, k = 1, \ldots, K, \quad (3)$$

where $R_k = \sum_{n=1}^{N} \gamma_{nk}$, and $\gamma_{nk} := \frac{\pi_k \mathcal{N}(x_n|\mu_k,\sigma_k)}{\sum_j \pi_j \mathcal{N}(x_n|\mu_j,\sigma_j)}$.

# The EM algorithm

$\mathrm{EM}(X), X = \{x_1, \ldots, x_n\}$

choose $K$ initial means, variances, and mixing coefficients $\mu_k, \sigma_k^2, \pi_k, i = 1, \ldots, K$;

**repeat**

for all $n = 1, \ldots, N, k = 1 \ldots, K$ set $\gamma_{nk} := \frac{\pi_k \mathcal{N}(x_n|\mu_k,\sigma_k)}{\sum_j \pi_j \mathcal{N}(x_n|\mu_j,\sigma_j)}$;

for $k = 1, \ldots K$ set $\mu_k^{new} := \frac{1}{R_k} \sum_n \gamma_{nk} x_n$,
$\sigma_k^{2new} := \frac{1}{R_k} \sum_n \gamma_{nk} (x_n - \mu_k^{new})^2, R_k := \sum_n \gamma_{nk}, \pi_k^{new} := \frac{R_k}{N}$;

**until** *convergence*;

**return** $\mu_k, \sigma_k^2, \pi_k, k = 1, \ldots, K$

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*convergence:* quality of solution no longer improves

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for all $n = 1, \ldots, N, k = 1 \ldots, K$ set $\gamma_{nk} := \frac{\pi_k \mathcal{N}(x_n | \mu_k, \sigma_k)}{\sum_j \pi_j \mathcal{N}(x_n | \mu_j, \sigma_j)}$;

```
/* maximization step */
```

for $k = 1, \ldots K$ set $\mu_k^{new} := \frac{1}{R_k} \sum_n \gamma_{nk} x_n$, $\sigma_k^{2new} := \frac{1}{R_k} \sum_n \gamma_{nk} (x_n - \mu_k^{new})^2, R_k := \sum_n \gamma_{nk}, \pi_k^{new} := \frac{R_k}{N}$;

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*convergence:* quality of solution no longer improves k-MEANS($P$)

```
choose k initial centroids c_1, ..., c_k;
repeat
    /* assignment step                                        */
    for i = 1, ..., k do
        C_i := set of points in P closest to c_i;
    end
    /* estimation step                                        */
    for i = 1, ..., k do
        c_i := c(C_i) = 1/|C_i| ∑_{p∈C_i} p;
    end
until convergence;
return c_1, ..., c_k and C_1, ..., C_k
```

Where: $C_i :=$ set of points in $P$ closest to $c_i$; $c_i := c(C_i) = \frac{1}{|C_i|} \sum_{p \in C_i} p$

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