

# Math Camp

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# Multivariate Optimization

## Optimizing multivariate functions

- Parameters  $\beta = (\beta_1, \beta_2, \dots, \beta_n)$  such that  $f(\beta|\mathbf{X}, \mathbf{Y})$  is maximized
- Policy  $\mathbf{x} \in \mathbb{R}^n$  that maximizes  $U(\mathbf{x})$
- Weights  $\pi = (\pi_1, \pi_2, \dots, \pi_K)$  such that a weighted average of forecasts  $\mathbf{f} = (f_1, f_2, \dots, f_k)$  have minimum loss

$$\min_{\pi} = -\left(\sum_{j=1}^K \pi_j f_j - y\right)^2$$

Today we'll describe analytic and computational approaches to optimization

- Analytic recipe for optimization
- Computational optimization
  - Multivariate Newton-Raphson
  - BFGS
  - Approximate Optimization: k-means

# Multivariate Optimization

## Definition

Let  $\mathbf{x} \in \mathbb{R}^n$  and let  $\delta > 0$ . Define a *neighborhood* of  $\mathbf{x}$ ,  $B(\mathbf{x}, \delta)$ , as the set of points such that,

$$B(\mathbf{x}, \delta) = \{\mathbf{y} \in \mathbb{R}^n : \|\mathbf{x} - \mathbf{y}\| < \delta\}$$

## Definition

Suppose  $f : X \rightarrow \mathbb{R}$  with  $X \subset \mathbb{R}^n$ . A vector  $\mathbf{x}^* \in X$  is a *global maximum* if, for all other  $\mathbf{x} \in X$

$$f(\mathbf{x}^*) > f(\mathbf{x})$$

A vector  $\mathbf{x}^{local}$  is a *local maximum* if there is a neighborhood around  $\mathbf{x}^{local}$ ,  $Q \subset X$  such that, for all  $\mathbf{x} \in Q$ ,

$$f(\mathbf{x}^{local}) > f(\mathbf{x})$$

# Multivariate Optimization

## Definition

A set  $X \subset \mathbb{R}^n$  is **compact** if it is closed and bounded

## Theorem

**Multivariate Extreme Value Theorem** Suppose  $f : X \rightarrow \mathbb{R}$  be continuous and  $X \subset \mathbb{R}^n$  and  $X$  compact. Then  $f$  takes on its **maximum** and **minimum** values on  $X$ .

We're going to come up with the multivariate equivalent of the **first order** and **second order** conditions now

# Gradient

## Definition

*Suppose  $f : X \rightarrow \mathbb{R}^n$  with  $X \subset \mathbb{R}^1$  is a differentiable function. Define the gradient vector of  $f$  at  $\mathbf{x}_0$ ,  $\nabla f(\mathbf{x}_0)$  as,*

$$\nabla f(\mathbf{x}_0) = \left( \frac{\partial f(\mathbf{x}_0)}{\partial x_1}, \frac{\partial f(\mathbf{x}_0)}{\partial x_2}, \frac{\partial f(\mathbf{x}_0)}{\partial x_3}, \dots, \frac{\partial f(\mathbf{x}_0)}{\partial x_n} \right)$$

# Gradient First Order Condition

## Theorem

Suppose  $f : X \rightarrow \mathbb{R}^1$ ,  $X \subset \mathbb{R}^n$ . Suppose  $\mathbf{a} \in X$  is a *local* extremum. Then,

$$\begin{aligned}\nabla f(\mathbf{a}) &= \mathbf{0} \\ &= (0, 0, \dots, 0)\end{aligned}$$

- Proof (intuition): same as one dimensional case (left-hand, right hand), just do it dimension by dimension
- **Critical Values:**
  - 1) Maximum
  - 2) Minimum
  - 3) **Saddle point**
- **Second Derivative Test!**

# Second Order Conditions: Hessian

## Definition

Suppose  $f : X \rightarrow \mathbb{R}^1$ ,  $X \subset \mathbb{R}^n$ , with  $f$  a twice differentiable function. We will define the **Hessian** matrix as the matrix of second derivatives at  $\mathbf{x}^* \in X$ ,

$$H(f)(\mathbf{x}^*) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(\mathbf{x}^*) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(\mathbf{x}^*) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(\mathbf{x}^*) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(\mathbf{x}^*) & \frac{\partial^2 f}{\partial x_2 \partial x_2}(\mathbf{x}^*) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n}(\mathbf{x}^*) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1}(\mathbf{x}^*) & \frac{\partial^2 f}{\partial x_n \partial x_2}(\mathbf{x}^*) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n}(\mathbf{x}^*) \end{pmatrix}$$

**General test**  $\rightsquigarrow$  Two Dimensional Test  $\rightsquigarrow$  Example

# Hessians

## Definition

Consider  $n \times n$  matrix  $\mathbf{A}$ . If, for all  $\mathbf{x} \in \mathbb{R}^n$  where  $\mathbf{x} \neq 0$ :

$$\mathbf{x}' \mathbf{A} \mathbf{x} > 0 \text{ } \mathbf{A} \text{ is positive definite}$$

$$\mathbf{x}' \mathbf{A} \mathbf{x} < 0 \text{ } \mathbf{A} \text{ is negative definite}$$

If  $\mathbf{x}' \mathbf{A} \mathbf{x} > 0$  for some  $\mathbf{x}$  and  $\mathbf{x}' \mathbf{A} \mathbf{x} < 0$  for other  $\mathbf{x}$ , then we say  $\mathbf{A}$  is *indefinite*



# Approximating functions and second order conditions

## Theorem

**Taylor's Theorem** Suppose  $f : \mathbb{R} \rightarrow \mathbb{R}$ ,  $f(x)$  is infinitely differentiable function. Then, the taylor expansion of  $f(x)$  around  $a$  is given by

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n$$

# Example Function

Suppose  $a = 0$  and  $f(x) = e^x$ . Then,

$$\begin{aligned}f'(x) &= e^x \\f''(x) &= e^x \\&\vdots \\f^n(x) &= e^x\end{aligned}$$

This implies

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} \dots + \frac{x^n}{n!} + \dots$$

# Multivariate Taylor's Theorem

## Theorem

*Suppose  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is a three-times continuously differentiable function, then around  $\mathbf{a} \in \mathbb{R}^n$ ,*

$$f(\mathbf{x}) = f(\mathbf{a}) + \nabla f(\mathbf{a})(\mathbf{x} - \mathbf{a}) + \frac{1}{2}(\mathbf{x} - \mathbf{a})' \mathbf{H}(f)(\mathbf{a})(\mathbf{x} - \mathbf{a}) + R(\mathbf{a}, \mathbf{x})$$

*where  $\frac{R(\mathbf{x}, \mathbf{a})}{\|\mathbf{x} - \mathbf{a}\|^2} \rightarrow 0$  as  $\mathbf{x} \rightarrow \mathbf{a}$*

# Intuition for Quadratic Form

Suppose  $\mathbf{x}^*$  is some critical value,

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*) + (\mathbf{x} - \frac{1}{2}\mathbf{x}^*)\mathbf{H}(f)(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*) + R(\mathbf{x}^*, \mathbf{x})$$

$$f(\mathbf{x}) - f(\mathbf{x}^*) = 0(\mathbf{x} - \mathbf{x}^*) + (\mathbf{x} - \frac{1}{2}\mathbf{x}^*)\mathbf{H}(f)(\mathbf{x}^*)(\mathbf{x} - \mathbf{x}^*) + R(\mathbf{x}^*, \mathbf{x})$$

For  $\mathbf{x}$  near  $\mathbf{x}^*$ ,  $R(\mathbf{x}^*, \mathbf{x}) \approx 0$

$\mathbf{H}(f)(\mathbf{x}^*)$  positive definite  $\rightarrow f(\mathbf{x}) > f(\mathbf{x}^*) \rightarrow$  local minimum

$\mathbf{H}(f)(\mathbf{x}^*)$  negative definite  $\rightarrow f(\mathbf{x}) < f(\mathbf{x}^*) \rightarrow$  local maximum

## Theorem

### *Second Derivative Test*

- If  $\mathbf{H}(f)(\mathbf{a})$  is *positive definite* then  $\mathbf{a}$  is a local minimum
- If  $\mathbf{H}(f)(\mathbf{a})$  is *negative definite* then  $\mathbf{a}$  is a local maximum
- If  $\mathbf{H}(f)(\mathbf{a})$  is *indefinite* then  $\mathbf{a}$  is a saddle point

# Second Derivative Test

Many ways to assess definiteness  $\rightsquigarrow$  use determinant

## Theorem

*Two Dimensional, Second Derivative Test.* Suppose  $f : X \rightarrow \mathbb{R}$  with  $X \subset \mathbb{R}^2$  and  $f$  twice differentiable. Write the **Hessian** of  $f$  at a critical value  $\mathbf{a}$ ,

$$\mathbf{H}(f)(\mathbf{a}) = \begin{pmatrix} A & B \\ B & C \end{pmatrix}$$

Then, we can conduct the second derivative test as:

- $AC - B^2 > 0$  and  $A > 0 \rightsquigarrow$  **positive definite**  $\rightsquigarrow \mathbf{a}$  is a local minimum
- $AC - B^2 > 0$  and  $A < 0 \rightsquigarrow$  **negative definite**  $\rightsquigarrow \mathbf{a}$  is a local maximum
- $AC - B^2 < 0 \rightsquigarrow$  **indefinite**  $\rightsquigarrow$  saddle point
- $AC - B^2 = 0$  **inconclusive**

# Multivariate Recipe

- 1) Calculate **gradient**
- 2) Set equal to zero, solve system of equations
- 3) Calculate **Hessian**
- 4) Assess **Hessian** at critical values
- 5) **Boundary values?** (if relevant)

# Example 1: A Simple Optimization Problem

Suppose  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  with

$$f(x_1, x_2) = 3(x_1 + 2)^2 + 4(x_2 + 4)^2$$

Calculate gradient

$$\nabla f(\mathbf{x}) = (6x_1 + 12, 8x_2 + 32)$$

$$\mathbf{0} = (6x_1^* + 12, 8x_2^* + 32)$$

We now solve the system of equations to yield  $x_1^* = -2$  and  $x_2^* = -4$



## Example 1: A Simple Optimization Problem

$$\mathbf{H}(f)(\mathbf{x}^*) = \begin{pmatrix} 6 & 0 \\ 0 & 8 \end{pmatrix}$$

$\det(\mathbf{H}(f)(\mathbf{x}^*)) = 48$  and  $6 > 0$  so  $\mathbf{H}(f)(\mathbf{x}^*)$  is positive definite. **local minimum**

## Example 2: Two Dimensional Ideal Points

Suppose legislators are considering legislation  $\mathbf{x} \in \mathbb{R}^2$ . And suppose legislator  $i$  has utility function  $U_i : \mathbb{R}^2 \rightarrow \mathbb{R}$ ,

$$U(\mathbf{x})_i = -(x_1 - \mu_1)^2 - (x_2 - \mu_2)^2$$

What is legislator  $i$ 's **optimal** policy?

$$\nabla f(\mathbf{x}) = (-2(x_1 - \mu_1), -2(x_2 - \mu_2))$$

$$\nabla f(\mathbf{x}) = \mathbf{0}$$

$$-2(x_1^* - \mu_1) = 0$$

$$-2(x_2^* - \mu_2) = 0$$

Solving yields  $x_1^* = \mu_1$  and  $x_2^* = \mu_2$ .

## Example 2: Two Dimensional Ideal Points

$$U(\mathbf{x})_i = -(x_1 - \mu_1)^2 - (x_2 - \mu_2)^2$$

Call  $\boldsymbol{\mu} = (\mu_1, \mu_2)$

The Hessian at the critical value is

$$\begin{aligned} \mathbf{H}(f)(\boldsymbol{\mu}) &= \begin{pmatrix} \frac{\partial^2 U_i}{\partial x_1 \partial x_1}(\boldsymbol{\mu}) & \frac{\partial^2 U_i}{\partial x_1 \partial x_2}(\boldsymbol{\mu}) \\ \frac{\partial^2 U_i}{\partial x_2 \partial x_1}(\boldsymbol{\mu}) & \frac{\partial^2 U_i}{\partial x_2 \partial x_2}(\boldsymbol{\mu}) \end{pmatrix} \\ &= \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix} \end{aligned}$$

So,  $-2 * -2 - 0 = 4 > 0$  and  $-2 < 0 \rightsquigarrow$  **negative definite**, maximum  $\boldsymbol{\mu} = (\mu_1, \mu_2)$  are legislator  $i$ 's two dimensional ideal point.

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Our task:

- Obtain likelihood (summary estimator)
- Derive maximum likelihood estimators for  $\mu$  and  $\sigma^2$
- Characterize sampling distribution

# Example 3: Maximum Likelihood Estimation, Normal Distribution

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$$L(\mu, \sigma^2 | \mathbf{Y}) \propto \prod_{i=1}^n f(Y_i | \mu, \sigma^2)$$

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Taking the logarithm, we have

$$l(\mu, \sigma^2 | \mathbf{Y}) = -\sum_{i=1}^n \frac{(Y_i - \mu)^2}{2\sigma^2} - \frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) + \textcolor{red}{c}$$

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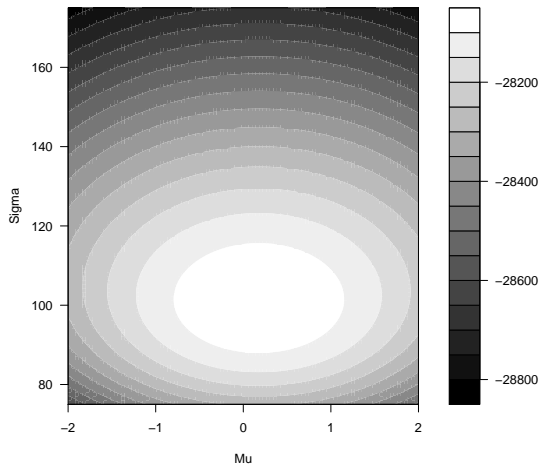
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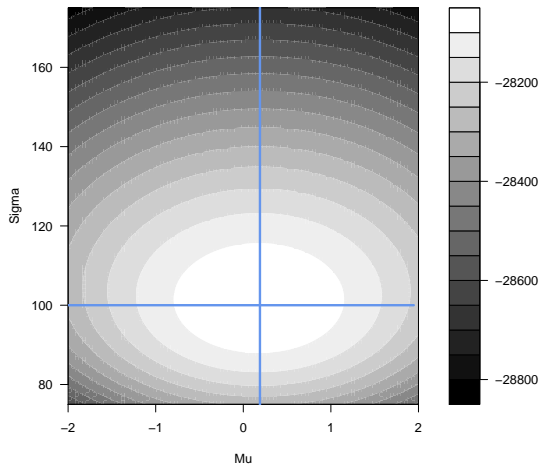
$$Y_i \sim \text{Normal}(0.25, 100)$$

- Used realized values  $y_i$  evaluate  $l(\mu, \sigma^2 | \mathbf{y})$

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Let's find  $\hat{\mu}$  and  $\hat{\sigma}^2$  that maximizes log-likelihood.



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Let's find  $\hat{\mu}$  and  $\hat{\sigma}^2$  that maximizes log-likelihood.

$$l(\mu, \sigma^2 | \mathbf{Y}) = - \sum_{i=1}^n \frac{(Y_i - \mu)^2}{2\sigma^2} - \frac{n}{2} \log(\sigma^2) + c'$$

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$$\frac{\partial l(\mu, \sigma^2 | \mathbf{Y})}{\partial \mu} = \sum_{i=1}^n \frac{2(Y_i - \mu)}{2\sigma^2}$$

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$$\frac{\partial l(\mu, \sigma^2) | \mathbf{Y}}{\partial \mu} = \sum_{i=1}^n \frac{2(Y_i - \mu)}{2\sigma^2}$$

$$\frac{\partial l(\mu, \sigma^2) | \mathbf{Y}}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (Y_i - \mu)^2$$

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$$0 = -\sum_{i=1}^n \frac{2(Y_i - \hat{\mu})}{2\hat{\sigma}^2}$$

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Solving for  $\hat{\mu}$  and  $\hat{\sigma}^2$  yields,

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$$\hat{\mu} = \frac{\sum_{i=1}^n Y_i}{n}$$

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Solving for  $\hat{\mu}$  and  $\hat{\sigma}^2$  yields,

$$\begin{aligned}\hat{\mu} &= \frac{\sum_{i=1}^n Y_i}{n} \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y})^2\end{aligned}$$

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## Example 3: Maximum Likelihood Estimation, Normal Distribution

$$\mathbf{H}(f)(\hat{\mu}, \hat{\sigma}^2) = \begin{pmatrix} \frac{\partial^2 l(\mu, \sigma^2 | \mathbf{Y})}{\partial \mu^2} & \frac{\partial^2 l(\mu, \sigma^2 | \mathbf{Y})}{\partial \sigma^2 \partial \mu} \\ \frac{\partial^2 l(\mu, \sigma^2 | \mathbf{Y})}{\partial \sigma^2 \partial \mu} & \frac{\partial^2 l(\mu, \sigma^2 | \mathbf{Y})}{\partial^2 \sigma^2} \end{pmatrix}$$

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Taking derivatives and evaluating at MLE's yields,

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Taking derivatives and evaluating at MLE's yields,

$$\mathbf{H}(f)(\hat{\mu}, \hat{\sigma}^2) = \begin{pmatrix} \frac{-n}{\hat{\sigma}^2} & 0 \\ 0 & \frac{-n}{(\hat{\sigma}^2)^2} \end{pmatrix}$$

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Taking derivatives and evaluating at MLE's yields,

$$\mathbf{H}(f)(\hat{\mu}, \hat{\sigma}^2) = \begin{pmatrix} \frac{-n}{\hat{\sigma}^2} & 0 \\ 0 & \frac{-n}{(\hat{\sigma}^2)^2} \end{pmatrix}$$

$$\det(\mathbf{H}(f)(\hat{\mu}, \hat{\sigma}^2)) = n^2 / \hat{\sigma}^5 \text{ and } -n / \hat{\sigma}^2 < 0 \rightsquigarrow \text{maximum}$$

# Computational Optimization

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Analytic solutions: often hard.

Computational solutions: simplify. Trade offs

- Newton-Raphson: expensive
- BFGS: less expensive
- EM-like optimization: solve intractable problems, parallelizable

# Multivariate Newton Raphson

Suppose  $f : \Re^n \rightarrow \Re$ . Suppose we have guess  $\mathbf{x}_t$ .

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R Code



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$r_{ij}$  = Indicator, Document  $i$  assigned to cluster  $j$

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Notation. Representation of document  $i$ :

$$\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{iM})$$

# Specifying the Method

- 1) Assume Euclidean distance between objects.
- 2) **Objective function**

$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^N \sum_{j=1}^K r_{ij} \left( \sum_{m=1}^M (y_{im} - \mu_{km})^2 \right)$$

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Two observations:

- If  $K = N$   $f(\mathbf{r}^*, \boldsymbol{\mu}^*, \mathbf{y}) = 0$  (Minimum)
  - Each observation in own cluster
  - $\mu_i = y_i$
- If  $K = 1$ ,  $f(\mathbf{r}^*, \boldsymbol{\mu}^*, \mathbf{y}) = N \times \sigma^2$ 
  - Each observation in one cluster
  - Center: average of documents



# Specifying the Method

- 1) Assume Euclidean distance between objects
- 2) Objective function
- 3) Algorithm for optimization

Iterative algorithm, Each Iteration  $t$

- Conditional on  $\mu^{t-1}$  (from previous iteration), choose  $r^t$
- Conditional on  $r^t$ , choose  $\mu^t$

Repeat until convergence, measured as change in  $f$ .

$$\text{Change} = f(\mu^t, r^t, y) - f(\mu^{t-1}, r^{t-1}, y)$$

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$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^N \sum_{j=1}^K r_{ij} \left( \sum_{m=1}^M (y_{im} - \mu_{km})^2 \right)$$

Algorithm for estimation:

Begin: initialize  $\boldsymbol{\mu}_1^{t-1}, \boldsymbol{\mu}_2^{t-1}, \dots, \boldsymbol{\mu}_K^{t-1}$

Choose  $\mathbf{r}^t$

$$r_{ij}^t = \begin{cases} 1 & \text{if } j = \arg \min_k \sum_{m=1}^M (y_{im} - \mu_{km})^2 \\ 0 & \text{otherwise,} \end{cases}$$

In words: Assign each document  $\mathbf{y}_i$  to the closest center  $\boldsymbol{\mu}_k$

$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^N \sum_{j=1}^K r_{ij} \left( \sum_{m=1}^M (y_{im} - \mu_{km})^2 \right)$$

Conditional on  $\mathbf{r}^t$ , choose  $\boldsymbol{\mu}^t$

Let's focus on  $\boldsymbol{\mu}_k$

$$f(\mathbf{r}, \boldsymbol{\mu}_k, \mathbf{y})_k = \sum_{i=1}^N r_{ik} \left( \sum_{m=1}^M (y_{im} - \mu_{km})^2 \right)$$

Focus on just  $\mu_{km}$

$$f(\mathbf{r}, \mu_{km}, \mathbf{y})_{km} = \sum_{i=1}^N r_{ik}(y_{im} - \mu_{km})^2$$

Quadratic: take derivative, set equal to zero (second derivative test works)

$$\frac{\partial f(\mathbf{r}, \mu_{km}, \mathbf{y})_{km}}{\partial \mu_{km}} = -2 \sum_{i=1}^N r_{ik}(y_{im} - \mu_{km})$$

$$2 \sum_{i=1}^N r_{ik}(y_{im} - \mu_{km}^t) = 0$$

$$\sum_{i=1}^N r_{ik}y_{im} - \mu_{km}^t \sum_{i=1}^N r_{ik} = 0$$

$$\frac{\sum_{i=1}^N r_{ik}y_{im}}{\sum_{i=1}^N r_{ik}} = \mu_{km}^t$$

$$\mu_k^t = \frac{\sum_{i=1}^N r_{ik} \mathbf{y}_i}{\sum_{i=1}^N r_{ik}}$$

In words:

- $\mu_k^t$  is the average of documents assigned to the  $k^{\text{th}}$  cluster

### Algorithm, In Words

- Conditional on center estimates, assign documents to closest cluster centers
- Conditional on document assignments, cluster centers are averages of documents assigned to the cluster

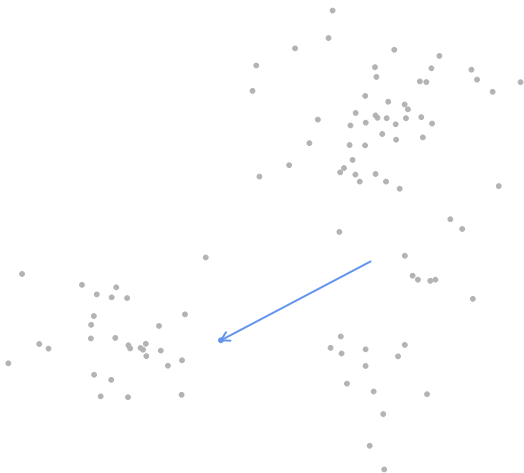
### Expectation-Maximization (EM) [connection guarantees convergence]

- Estimation of  $r \rightsquigarrow$  Expectation step (data augmentation)
- Estimation of  $\mu_k \rightsquigarrow$  Maximization Step

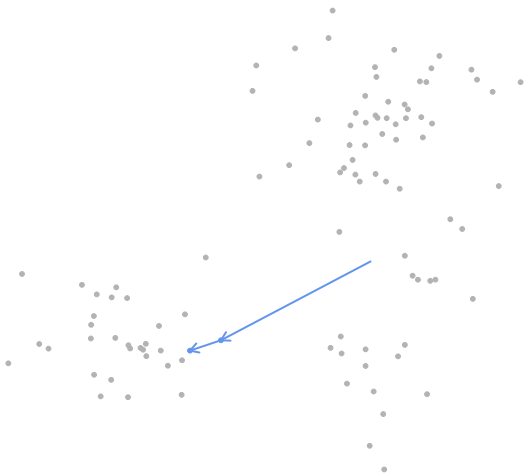
# Visual Example



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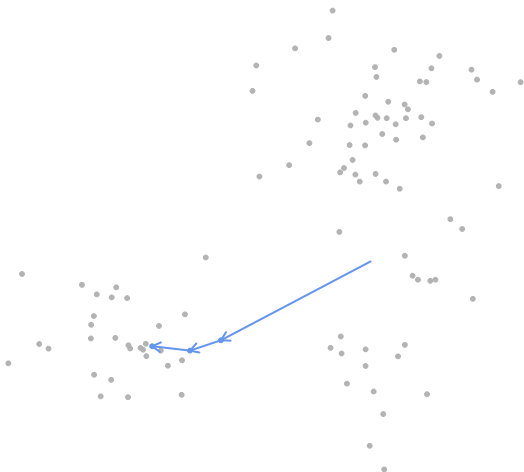


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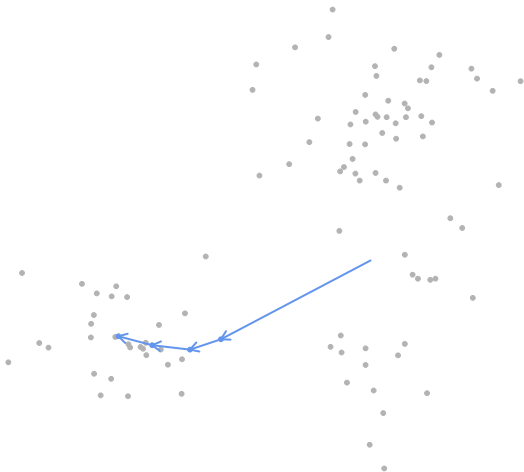




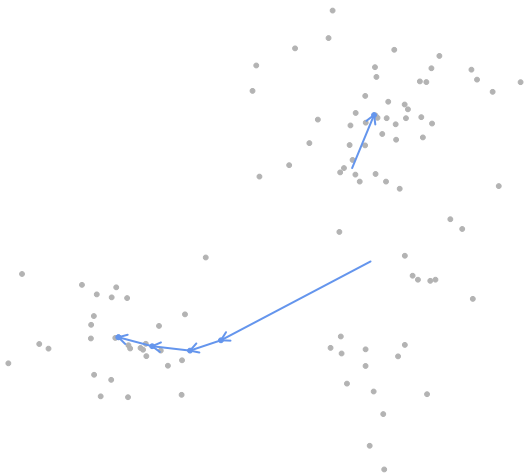
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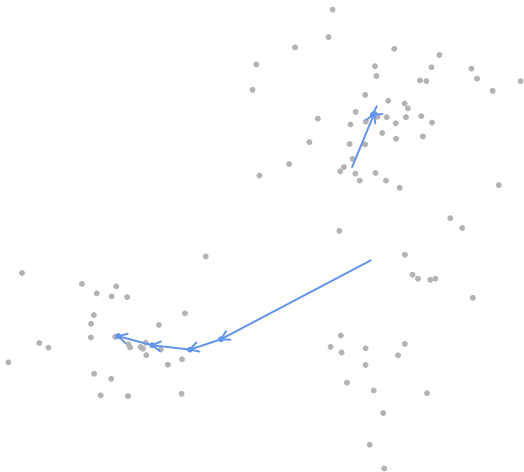
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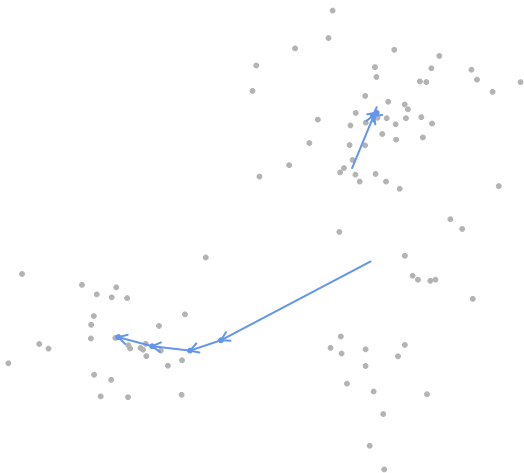
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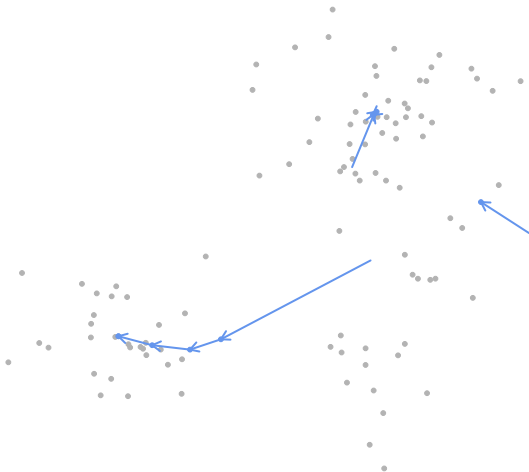
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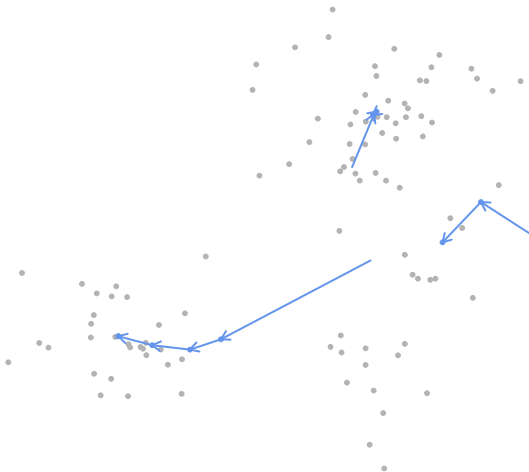
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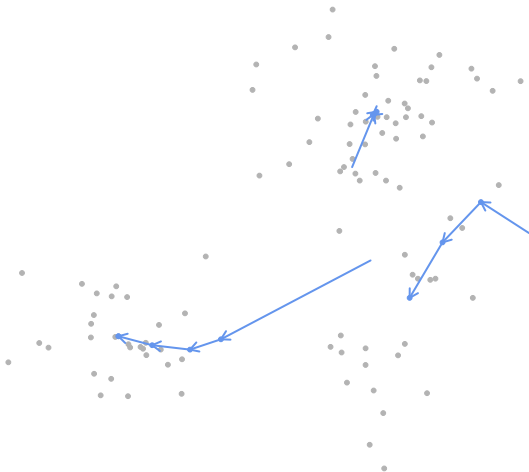
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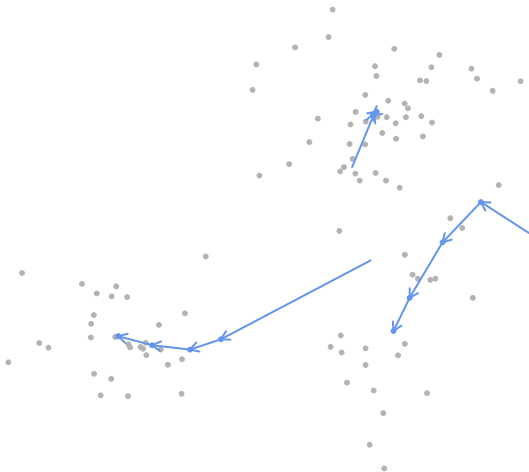


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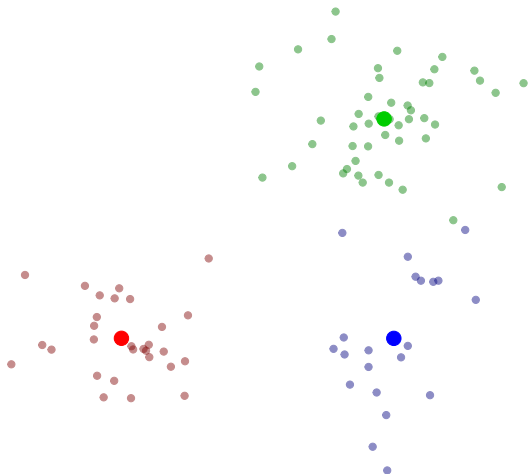




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## Genetic Optimization:

- Evaluate fitness of solutions
- Randomly select most fit, then combine
- Can converge to **global** maximum, but might require extensive run time

# Where We Are Going

- Done with math component
- Start probability tomorrow