Optimization

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What is optimization?

- From *Merriam-Webster*:
  - (noun) an act, process, or methodology of making something (such as a design, system, or decision) as fully perfect, functional, or effective as possible.
  - specifically : the mathematical procedures (such as finding the maximum of a function) involved in this

- A mathematical definition:
  - Given $f: A \to R$,
    find $\boldsymbol{x}^* \in A$
    such that $f(\boldsymbol{x})$ is minimized at $\boldsymbol{x} = \boldsymbol{x}^*$

(Note: maximization can be easily flipped to a minimization)

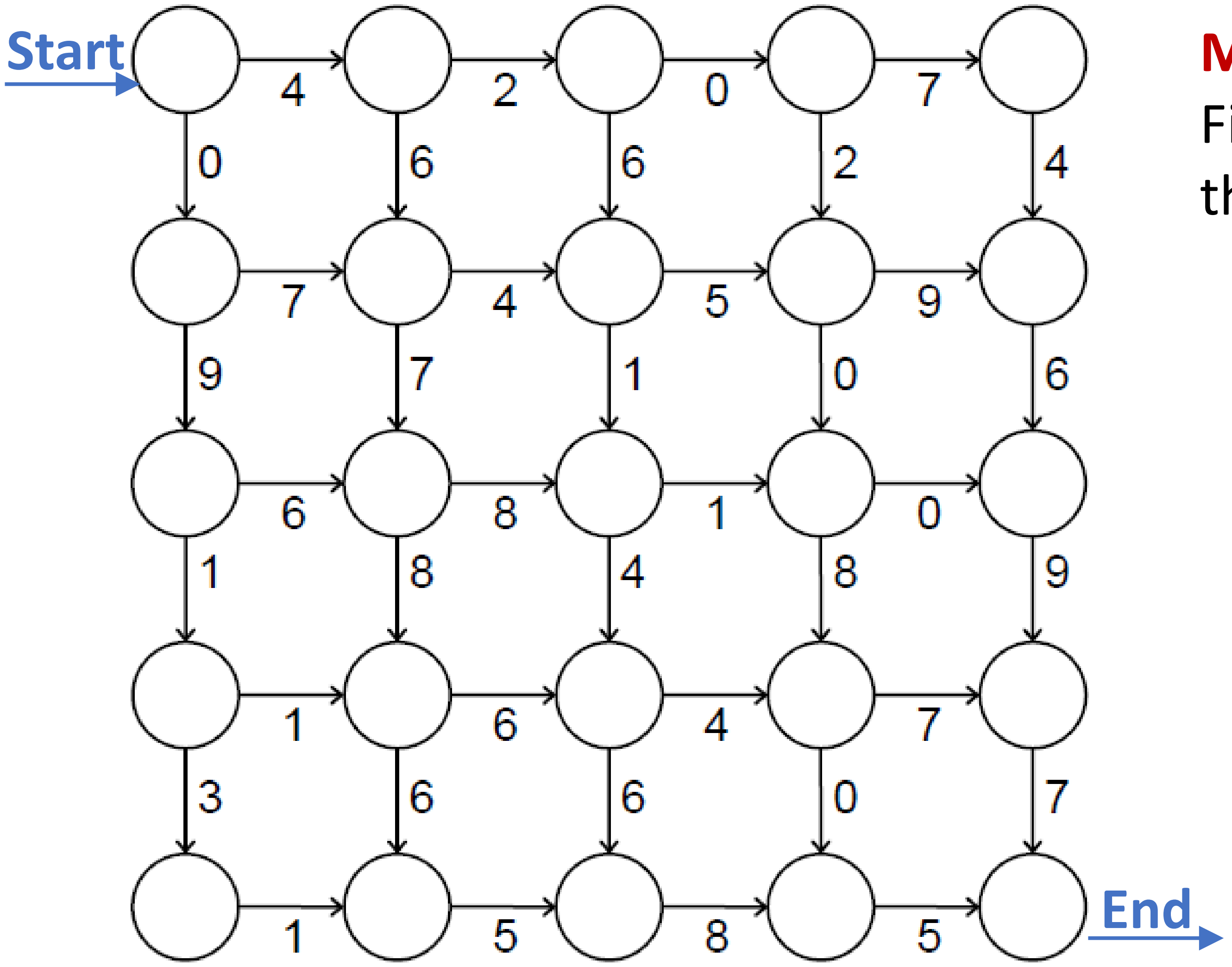
Numerical optimization : examples with closed-form solutions

- Unconstrained optimization
  - $f(x) = x^2 + 2x + 2$
  - $f(x) = (x+1)^2 + 1 \geq 1$ (equality holds at $x = -1$)

- Constrained optimization
  - $f(x) = x^2 + 2x + 2, \quad (x \geq 0)$
  - $f'(x) = 2x + 2 > 0$ when $x \geq 0$, so monotonically increasing.
  - $f(x)$ is minimized at $x = 0$, and $f(x) \geq 2$.

You are very lucky if your real-world optimization problem has a closed-form solution

Combinatorial optimization : an example



Manhattan Tourist Problem:
Find a path with
the minimum total cost.

Today, we will not cover combinatorial optimization

Mathematical optimization problem

- Minimize the objective function

$$f_0(\boldsymbol{x})$$

- subject to the constraints

$$f_i(\boldsymbol{x}) \leq b_i, \qquad i \in \{1,2,\cdots,m\}$$

- where
  - optimization variable $\boldsymbol{x} = (x_1, \cdots, x_n)$
  - objective function f_0: $\mathbb{R}^n \to \mathbb{R}$
  - constraint function f_i: $\mathbb{R}^n \to \mathbb{R}$, $i \in \{1, \cdots, m\}$

Why study optimization?

- It is important to formulate what you want as an optimization problem.

  (e.g. LASSO) Given $X \in \mathbb{R}^{n \times p}$, $\boldsymbol{y} \in \mathbb{R}^{n}$, and $\lambda \geq 0$,

  We want to find $\boldsymbol{\beta} \in \mathbb{R}^{p}$ that minimizes

$$f(\boldsymbol{\beta}) = \|\boldsymbol{y} - X\boldsymbol{\beta}\|_2 + \lambda\|\boldsymbol{\beta}\|_1 = (\boldsymbol{y} - X\boldsymbol{\beta})^T(\boldsymbol{y} - X\boldsymbol{\beta}) + \lambda \sum_{i=1}^{p} |\beta_i|$$

- It is even more important find out how to solve the optimization problem.
  - This may not be a fun activity for everybody, but useful for most of us.

Types of optimization problems

- By type of solutions
  - Numerical optimization
  - Combinatorial optimization
- By number of variables
  - Single-dimensional optimization
  - Multi-dimensional optimization
- By randomness in algorithm
  - Deterministic optimization
  - Stochastic optimization
- By type of objective function
  - Convex optimization
  - Non-convex optimization
- By constraints
  - Constrained optimization
  - Unconstrained optimization
- By optimality of the solution
  - Local optimization
  - Global optimization

Optimization: three key questions

1. How can I formulate the problem into an optimization problem?
   - Articulate your problem in mathematical terms.
   - In some cases, you may not even have realized that it is an optimization problem.

2. Do I know how to obtain a solution for the optimization problem?
   - Having an objective function does not automatically solve the problem.
   - Certain optimization problems are much harder than others.

3. Do I know what the time complexity of the method I chose is?
   - If you have big data, time complexity is one of the key factor to consider.
   - The solution should be not only possible but also feasible to obtain.

Example: maximum likelihood estimation (MLE)

- Likelihood function
  - $\boldsymbol{x}$: observed data
  - $\boldsymbol{\theta}$: model parameter
  - $f(\boldsymbol{X} = \boldsymbol{x}; \boldsymbol{\theta})$: probability density (mass) function
  - $L(\boldsymbol{\theta}; \boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{\theta})$: likelihood function

- Maximum likelihood estimation (MLE) : find

$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} L(\boldsymbol{\theta}; \boldsymbol{x})$$

- MLE is a useful across many areas of statistical inference.

- MLE is an instance of mathematical optimization problems

Example: MLE in logistic regression

- Given
  - $\boldsymbol{y} \in \{-1,1\}^n$
  - $X \in \mathbb{R}^{n \times p}$
  - $\boldsymbol{\beta} \in \mathbb{R}^p$
- Likelihood function

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} \Pr(y_i = 1; X, \boldsymbol{\beta}) = \prod_{i=1}^{n} \frac{1}{1 + \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})}$$

- Log-likelihood function

$$l(\boldsymbol{\beta}) = \log L(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log\left(\frac{1}{1 + \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})}\right)$$

This is an unconstrained optimization problem

A simple 1-dimensional case

- Suppose that $p = 1$, then the log-likelihood function becomes

$$l(\beta) = \log L(\beta) = \sum_{i=1}^{n} \log \left[\frac{1}{1 + \exp(-y_i x_i \beta)} \right]$$

- Maximum likelihood estimate (MLE) is

$$\hat{\beta} = \arg\max_{\beta} \left(\sum_{i=1}^{n} \log \left[\frac{1}{1 + \exp(-y_i x_i \beta)} \right] \right)$$

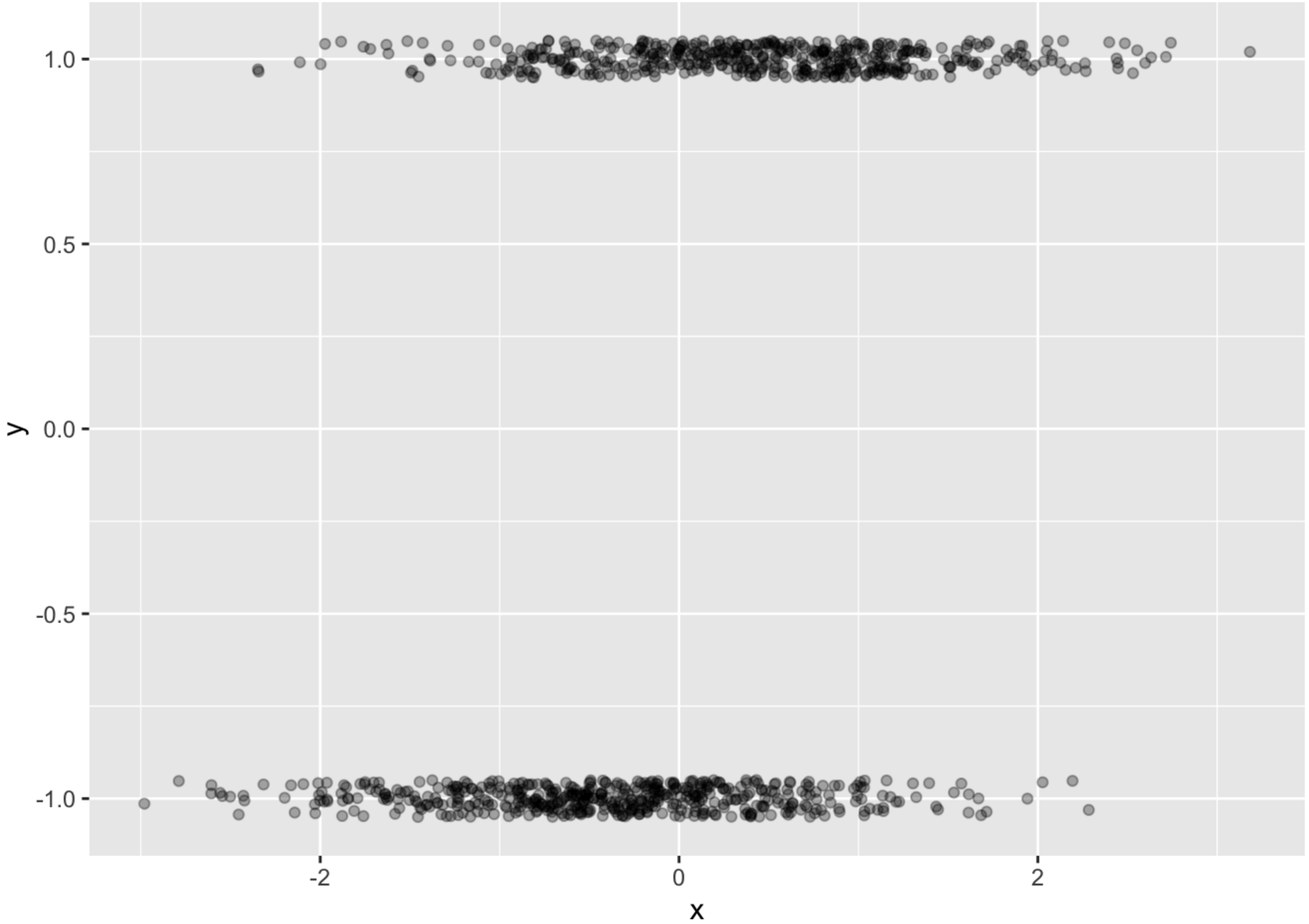
Q. Does a close-form solution exist?

Example : 1-d MLE in logistic regression

```
n <- 1000          # make 1,000 arbitrary example points
x <- rnorm(n)      # where x is normally distributed
y <- rbinom(n,1,1/(1+exp(-x))) * 2 - 1  # y follows univariate logisti
c model of x
df <- data.frame(x=x, y=y)
library(ggplot2)
ggplot(df,aes(x,y)) + geom_point(position=position_jitter(w=0,h=0.05),
alpha=0.3)
```

See the examples in the R markdown file in Canvas

Example data (jittered)

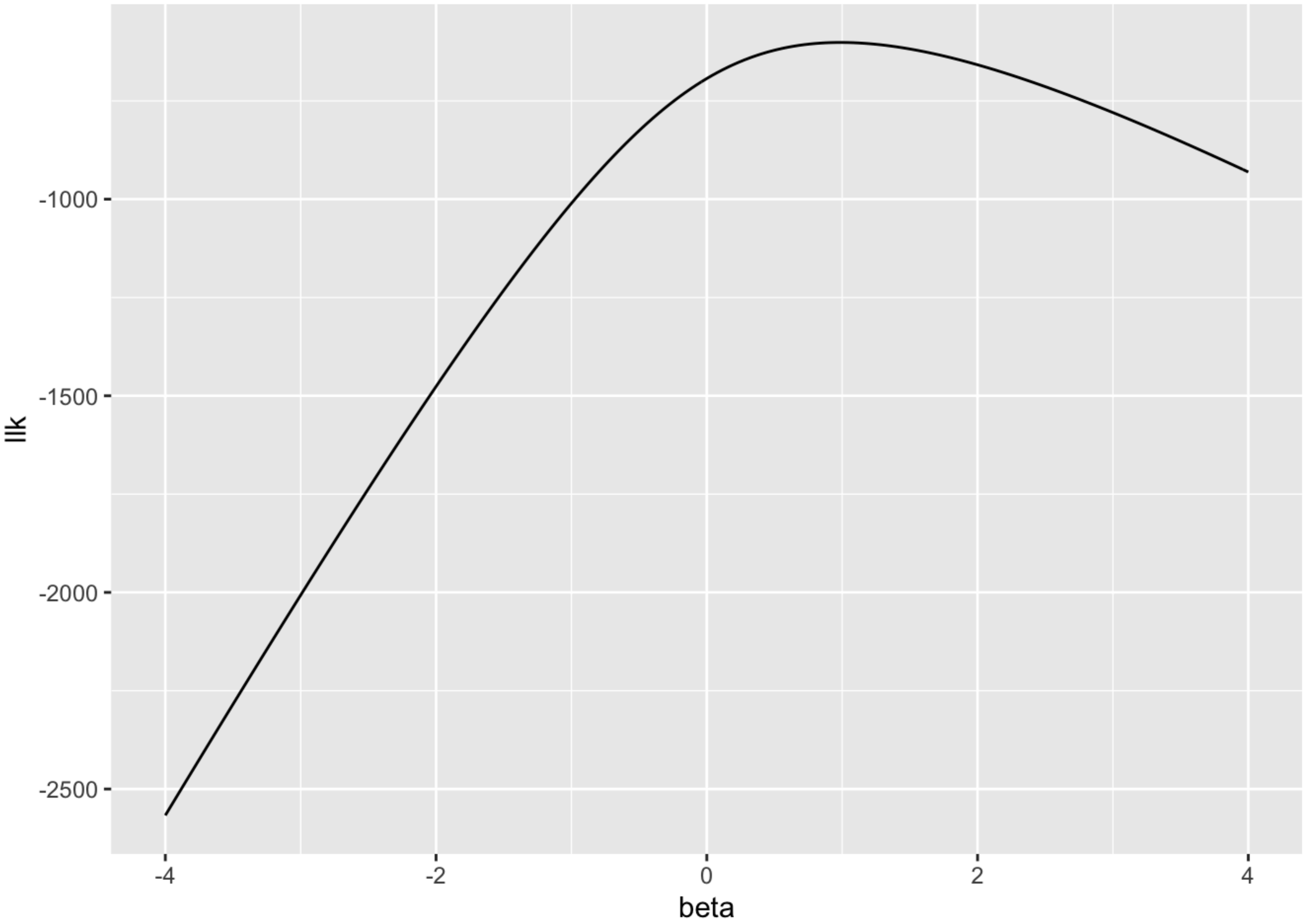


Likelihood function

$$l(\beta) = \log L(\beta) = \sum_{i=1}^{n} \log\left[\frac{1}{1+\exp(-y_i x_i \beta)}\right]$$

```
llk1 <- function(beta, x, y) {
  return( -sum(log(1+exp(0-y*x*beta))) )
}
betas <- (-100:100)/25
df <- data.frame(beta=betas,llk=sapply(betas,function(b) { llk1(b,x,y) }))
ggplot(df,aes(beta,llk)) + geom_line()
```

Visualization of the likelihood function



Single-dimensional optimization problem

- Given
  - $f(x)$: the objective function
  - We do not know how the function is shaped *a priori*.
  - Evaluation of $f(x)$ could be expensive – needs as few evaluations as possible.

- Want
  - Find x that minimizes $f(x)$
  - How difficult can this be?

Single-dimensional optimization could be tricky

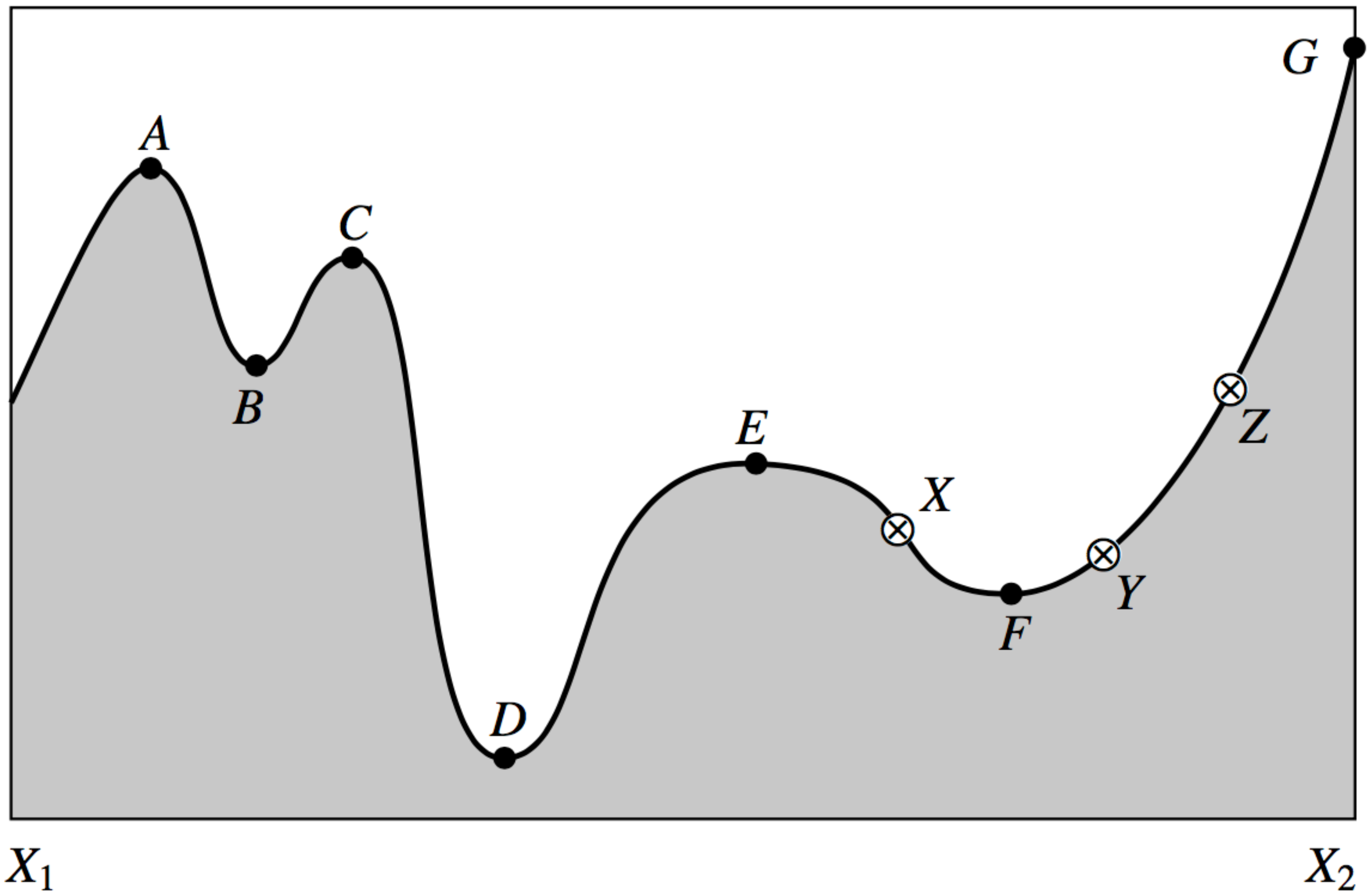


Image: Press WH, Teukosky SA, Vetterling W, Flannery BP (2007) Numerical Recipes, 3rd Edition, Cambridge University Press

Local vs. Global optimization

- **Globally optimal point**: $\boldsymbol{x}$ is globally optimal if

$$f_0(\boldsymbol{x}) = \inf_{\boldsymbol{z} \in \mathcal{X}} f_0(\boldsymbol{z})$$

where $\mathcal{X}$ is a set of values that satisfy the contraints

- **Locally optimal point**: $\boldsymbol{x}$ is locally optimal if there exists R > 0 such that

$$f_0(\boldsymbol{x}) = \inf_{|\boldsymbol{z}-\boldsymbol{x}| \leq R,\ \boldsymbol{z} \in \mathcal{X}} f_0(\boldsymbol{z})$$

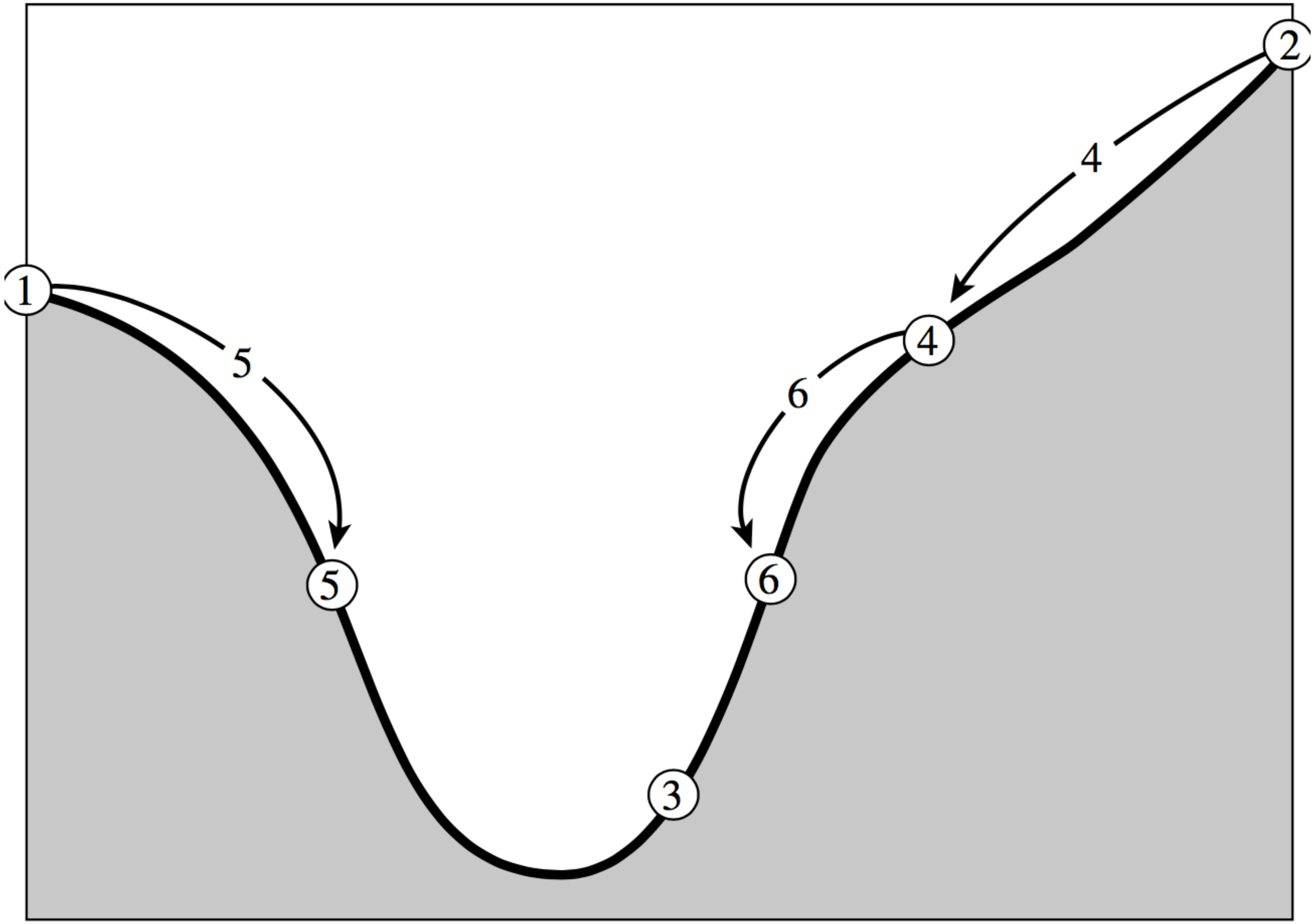
Bracketing: from global to local optimization

- The goal of bracketing is to find three points such that

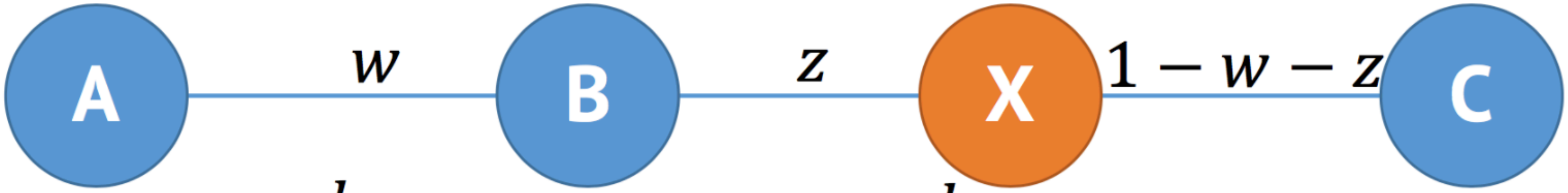
$$a < b < c$$
$$f(b) < f(a)$$
$$f(b) < f(c)$$

- Once such a, b, c are identified for a continuous function $f(\cdot)$, there should be at least one locally optimal point between a and c.

Golden section search



Minimizing the worst-case damage



$$w = \frac{b-a}{c-a} \qquad z = \frac{x-b}{c-a}$$

- The next interval will have length either $1 - w$ or $w + z$.
- Optimal condition must satisfy the following two conditions:
  - $1 - w = w + z$
  - $\frac{z}{1-w} = w$
- Solving the equations will lead to the golden ratio $w = \frac{3-\sqrt{5}}{2} = 0.38197$.
- This will guarantee that the interval size will reduce by ~38% at each step.

Algorithms for single-dimensional optimization

- Golden section search
  - At each iteration, the bracket size reduces by ~38%.
  - Guaranteed convergence, but could be slow.
- Parabola method
  - Approximate a quadratic function based on 3 points.
  - Often faster than golden search, but may not converge.
- Brent's method
  - Combination of parabola method and golden search.
  - Most widely used method for single-dimensional optimization.

Finding MLE using Brent's method

```r
## make sure to flip the sign of the objective function
## to convert the problem into miminization problem.
print(optimize(function(b) { 0-llk1(b, x, y)}, interval=c(-4,4)))
```

```
## $minimum
## [1] 0.9865495
##
## $objective
## [1] 601.4521
```

Multi-dimensional optimization

- More common type of optimization problems
  - Many variables need to be estimated together.

- A LOT harder than single-dimensional optimization
  - The search space is A LOT larger, especially for high-dimensions
  - Checking for local minimum is more complicated.
  - Checking for global minimum is even more complicated.

- A LOT more diversity in the available algorithms.

Ways to optimize multi-dimensional function

- If only the objective function is available (no gradient or Hessian)
  - Nelder-Mead algorithm

- If the objective function and gradient are available
  - Gradient descent (coordinate, batch, stochastic) algorithms
  - Quasi-Newton methods : BFGS or L-BFGS-B algorithms

- If objective function, gradient, and Hessian are available
  - Newton's method

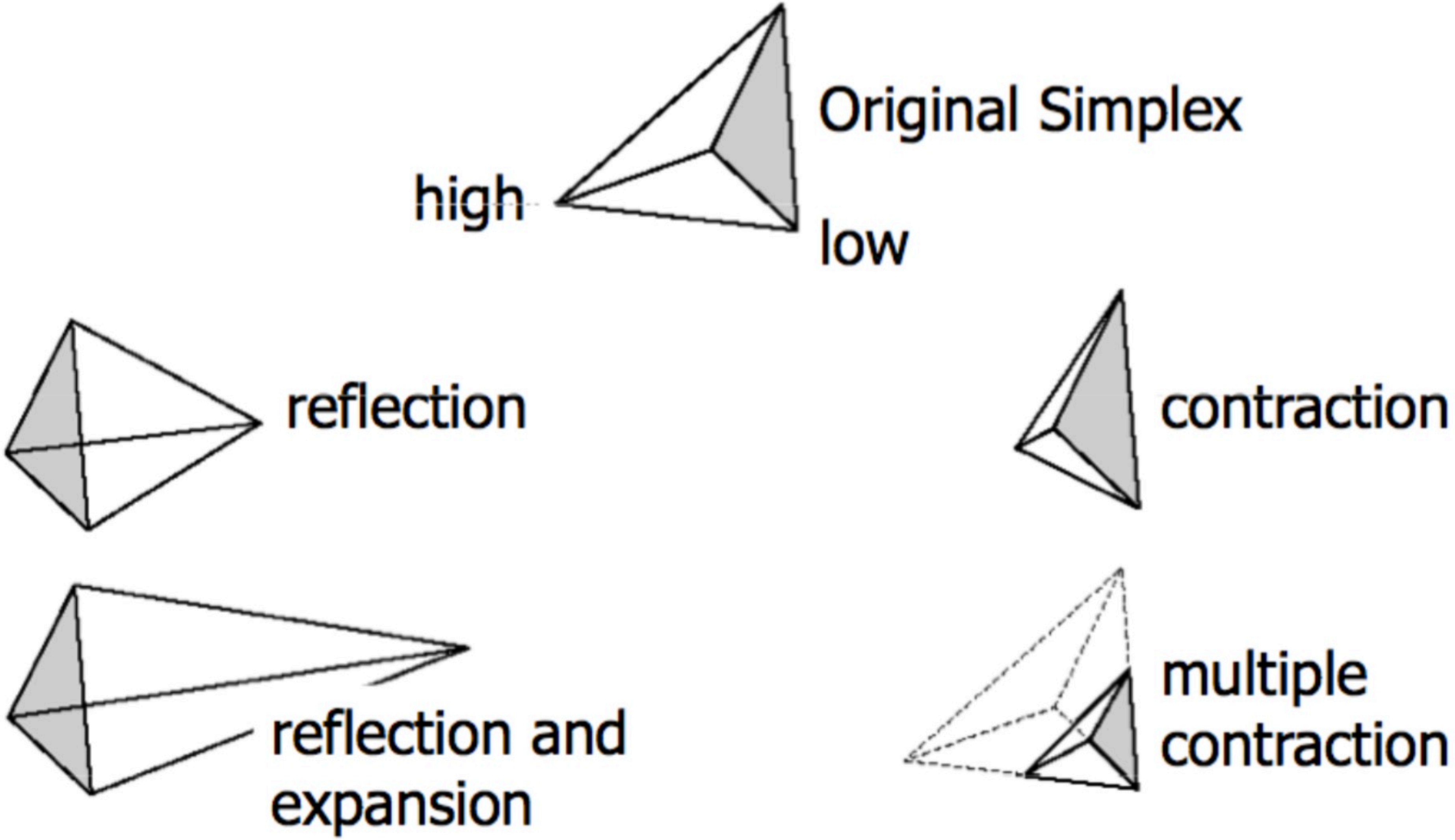
    but Hessian is expensive to compute for high-dimensions, so not very common.

These are generic methods, and many other context-specific methods are available

Nelder-Mead algorithm

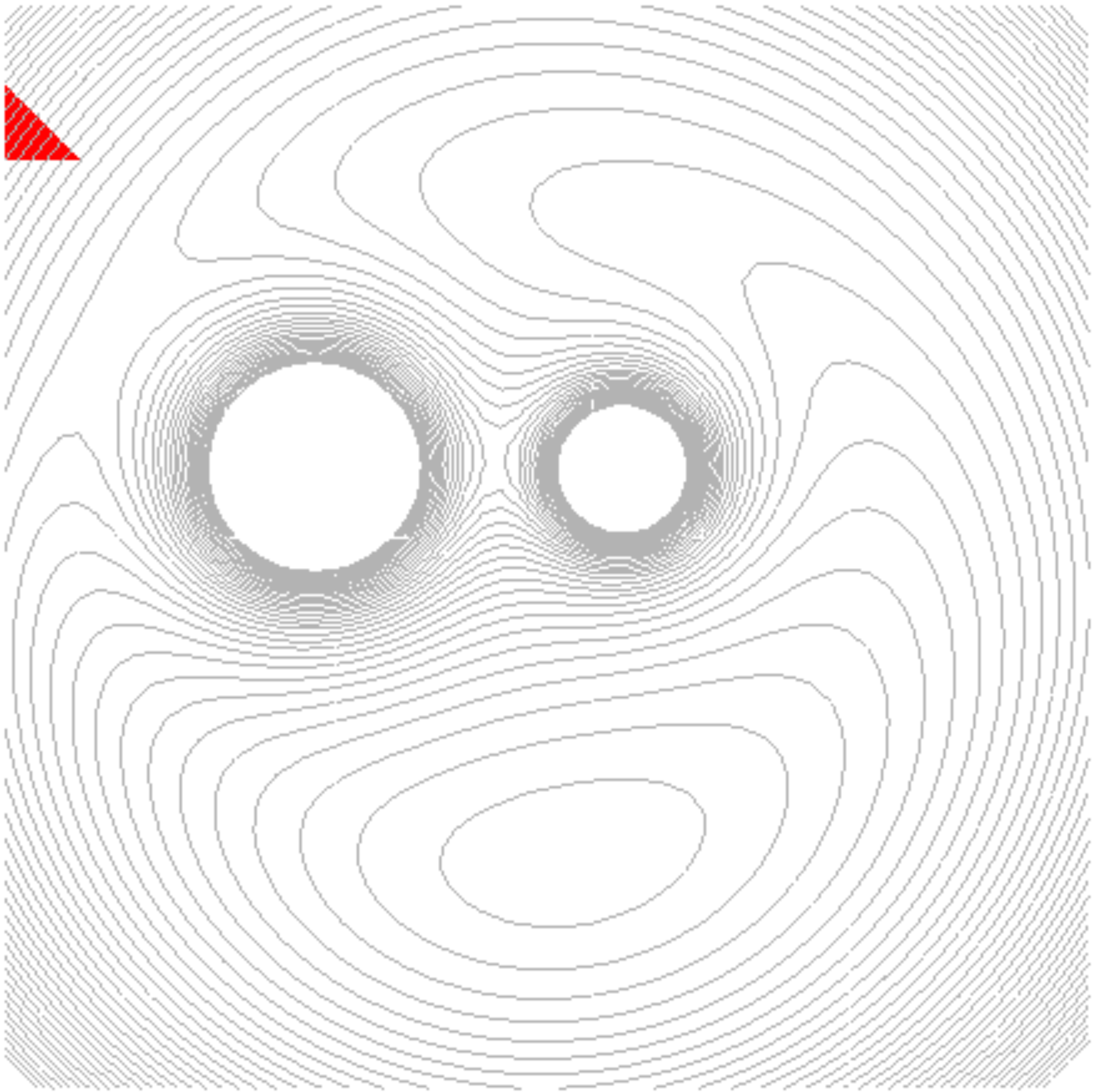
- A general-purpose multi-dimensional minimization method.
- Published in 1965, and cited >29,000 times to date.
- Simple to use - does not require derivatives.
- Works quite well in practice for low (e.g. several) dimensions.
- No theoretical guarantee for convergence (either local or global)
- Typically slower than other methods that leverage gradient.

Basic operations of Nelder-Mead algorithm



Press WH, Teukosky SA, Vetterling W, Flannery BP (2007) *Numerical Recipes, 3rd Edition,* Cambridge University Press

Illustration of Nelder-Mead Algorithm



https://userpages.umbc.edu/~rostamia/2017-09-math625/images/nelder-mead.gif

Example of multi-dimensional optimization

- Multi-dimensional logistic regression

$$l(\boldsymbol{\beta}) = \log L(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log\left(\frac{1}{1 + \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})}\right)$$

- A straightforward extension of the 1-d logistic regression

Example R code

```r
n <- 1000                          # make 1,000 arbitrary example points
beta <- c(0.3, 0.1, 0.03, 0, 0) # These are true effect sizes
p <- length(beta)                  # p is the dimension of the variables
X <- matrix(rnorm(n*p), n, p)    # X is a (n x p) matrix of predictor variables
y <- rbinom(n,1,1/(1+exp(0-X%*%beta))) * 2 - 1  # y is a size n vector of -1/1
```

Example of simulated data

```
head(X)
```

```
##              [,1]        [,2]        [,3]         [,4]        [,5]
## [1,]  0.4338128 -0.55187016  1.20380712 -1.302355079 -0.20147809
## [2,]  0.3658146  0.25108105  2.78898510  1.842643877  1.78737581
## [3,] -1.1087396  1.42582282 -0.09182399 -1.303832621  0.25927485
## [4,] -0.1451349 -0.06481368 -0.85645621 -0.939867038  0.95440592
## [5,]  0.3856186  0.25909865  0.88808601  0.755552557  0.65323539
## [6,] -0.6401423 -1.05290198 -1.59694764 -0.003498132  0.09643192
```

```
table(y)
```

```
## y
##  -1   1
## 469 531
```

Likelihood function

```
llk2 <- function(b, X, y) {
  return( -sum(log(1+exp(-y*(X%*%b)))) )
}

llk2(c(0,0,0,0,0), X, y)
```

```
## [1] -693.1472
```

Null likelihood

```
llk2(c(0.3,0.1,0.03,0,0), X, y)
```

```
## [1] -677.0216
```

Likelihood at the true parameter

Q. Is this the MLE?

Nelder-Mead is implemented in optim()

optim {stats} R Documentation

General-purpose Optimization

Description

General-purpose optimization based on Nelder–Mead, quasi-Newton and conjugate-gradient algorithms. It includes an option for box-constrained optimization and simulated annealing.

Usage

```
optim(par, fn, gr = NULL, ...,
      method = c("Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "SANN",
                 "Brent"),
      lower = -Inf, upper = Inf,
      control = list(), hessian = FALSE)

optimHess(par, fn, gr = NULL, ..., control = list())
```

Arguments

`par`	Initial values for the parameters to be optimized over.
`fn`	A function to be minimized (or maximized), with first argument the vector of parameters over which minimization is to take place. It should return a scalar result.
`gr`	A function to return the gradient for the `"BFGS"`, `"CG"` and `"L-BFGS-B"` methods. If it is `NULL`, a finite-difference approximation will be used. For the `"SANN"` method it specifies a function to generate a new candidate point. If it is `NULL` a default Gaussian Markov kernel is used.
`...`	Further arguments to be passed to `fn` and `gr`.
`method`	The method to be used. See 'Details'. Can be abbreviated.

Logistic MLE using Nelder-Mead algorithm

```
optim(c(0,0,0,0,0), function(b) { 0-llk2(b, X, y)})
```

```
## $par
## [1]  0.35057819  0.09064599 -0.03585259  0.10049316 -0.06493131
##
## $value
## [1] 674.4148
##
## $counts
## function gradient
##      312       NA
##
## $convergence
## [1] 0
##
## $message
## NULL
```

Optimization with gradients

- Gradient is a multivariate generalization of derivative

$$\nabla f_0(\boldsymbol{x}) = \left(\frac{\partial}{\partial x_1} f_0(\boldsymbol{x}), \ldots, \frac{\partial}{\partial x_p} f_0(\boldsymbol{x}) \right)$$

- For differentiable objective function, gradient is useful..
  - … to approximate the “slope” of the objective function.
  - … to reduce the number of function evaluations.
  - … to achieve better convergence properties.

Coordinate descent algorithm

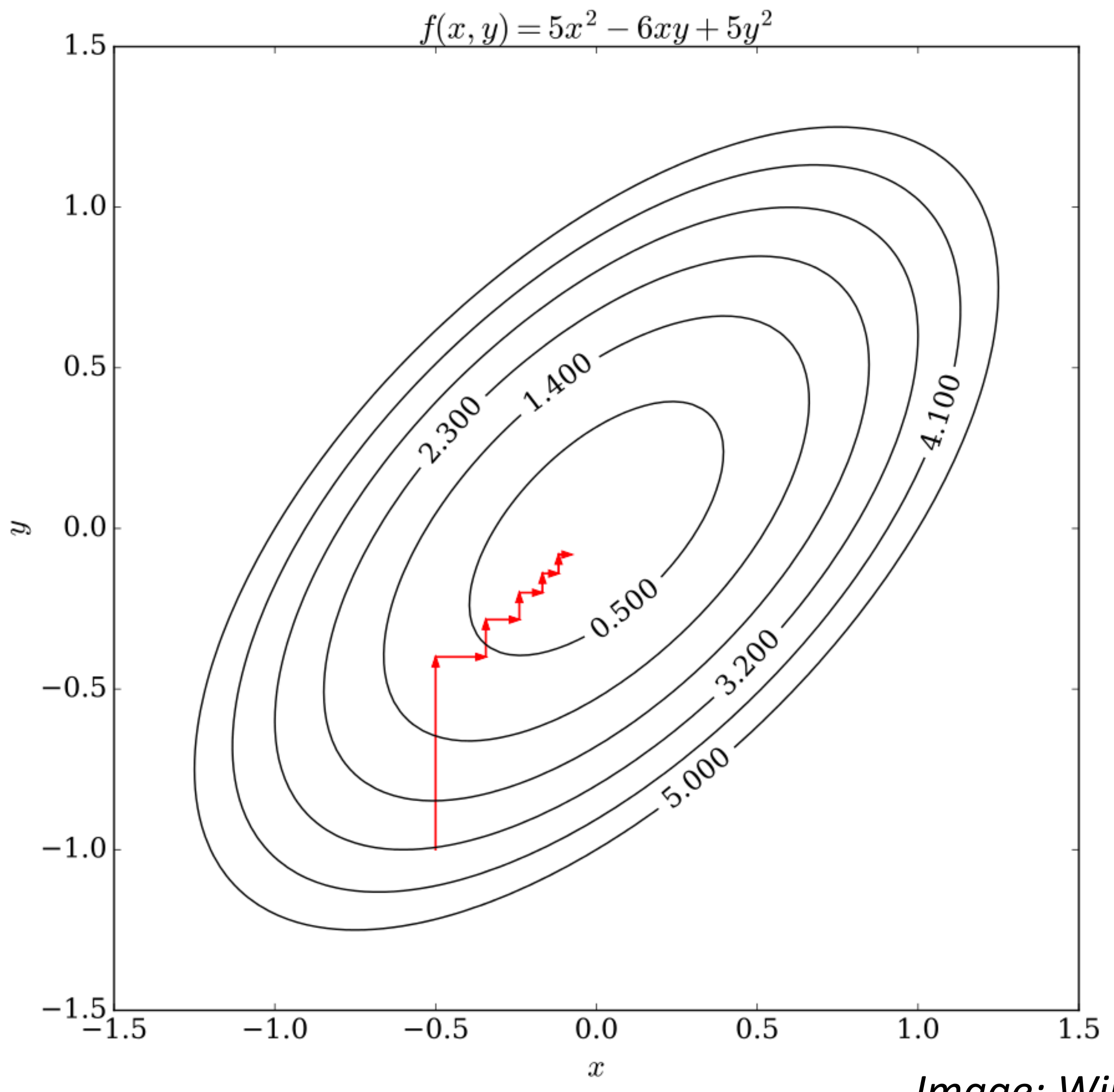
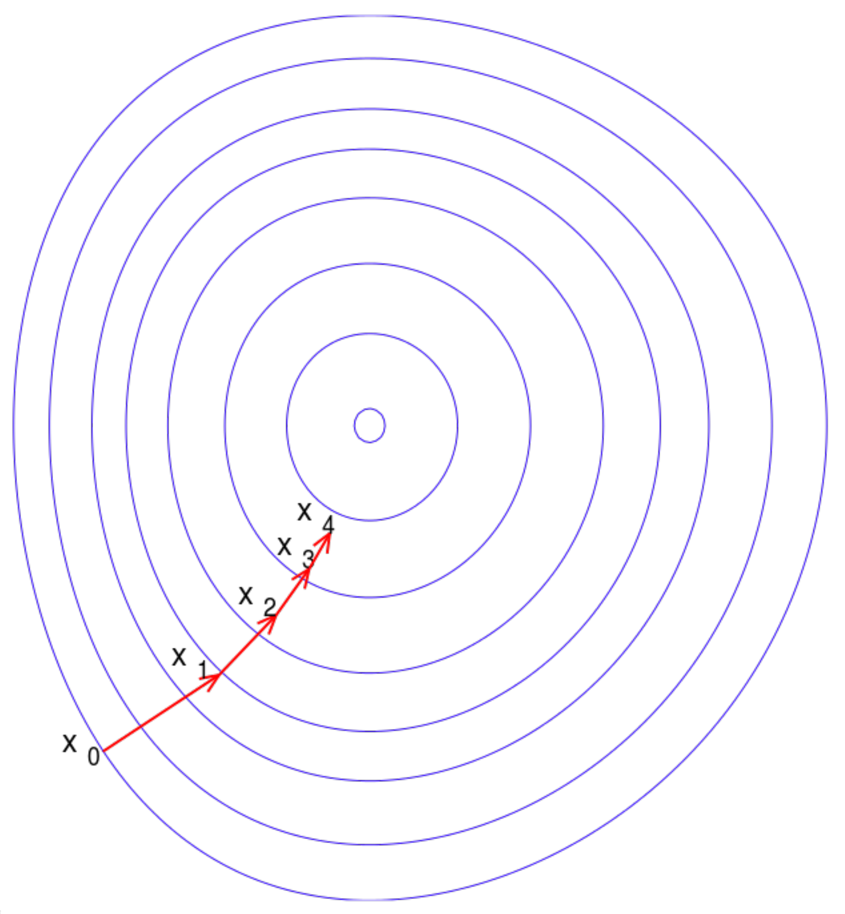


Image: Wikipedia

- Alternate each dimension for iterative update.
- Uses single-dimensional derivative to determine the direction and size of update.
- One of the simplest method.
- Does not work at all in some cases (where no improvement can be made using a single dimension).

Gradient descent algorithm



https://en.wikipedia.org/wiki/Gradient_descent

- Also called steepest descent algorithm.
- Parameters are updated to the direction proportional to the negative gradient of the objective function

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \gamma^{(t)} \nabla f_0(\boldsymbol{x}^{(t)})$$

- Choosing the step size is one of the tricky part in implementation

Stochastic gradient descent (SGD)

- For very large data, calculating gradient across all data can be time-consuming.
- In many cases, the object-function can be separated into a summation form

$$f_0(\boldsymbol{x}; D) = \sum_{i=1}^{m} f_0^{(i)}(\boldsymbol{x}; \boldsymbol{d}_i)$$

- Then, the gradient can also be represented into a summation form.

$$\nabla f_0(\boldsymbol{x}; D) = \sum_{i=1}^{m} \nabla f_0^{(i)}(\boldsymbol{x}; \boldsymbol{d}_i)$$

- Stochastic gradient descent compute gradient from partial data (single observation or mini-batch) to expedite the speed of update at the expense of smaller improvement at each update.

Types of gradient descent algorithms

- Batch gradient descent
  - Use all observations to compute gradient $\nabla f_0(\boldsymbol{x}^{(t);D})$
  - Takes longer to compute, but gives a right direction to update parameters.
- Stochastic gradient descent
  - Update the parameters using a single-sample gradient $\nabla f_0^{(i)}(\boldsymbol{x}^{(t,i)}; \boldsymbol{d}_i)$
  - Gradient can be computed faster, but update can go in a wrong direction.
- Mini-batch gradient descent
  - Compute gradient using a small batch of samples.
  - Gradient is more informative than using only a single sample, at the expense of increased cost of computation.

Stochastic gradient descent - Illustration

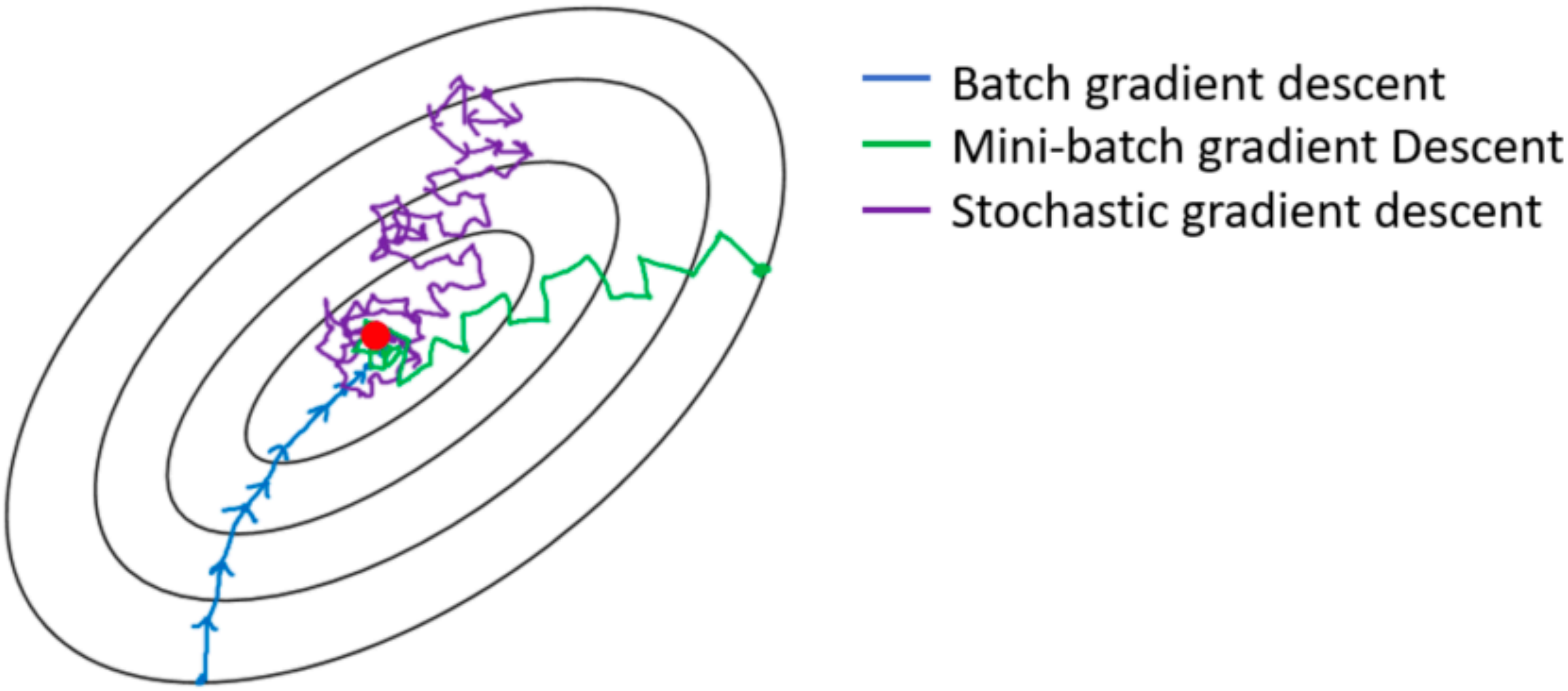
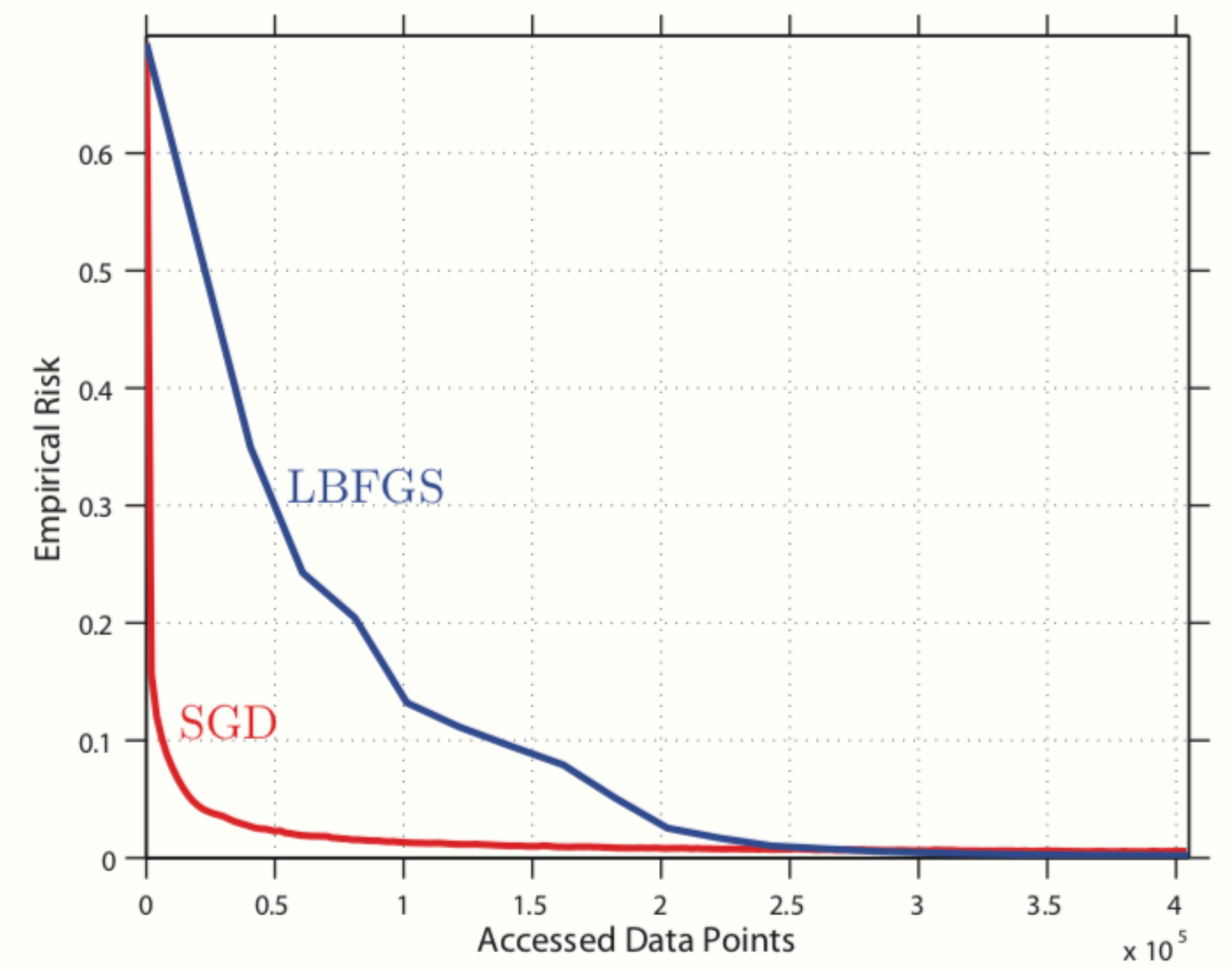


Image by Imad Dabbura from towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3

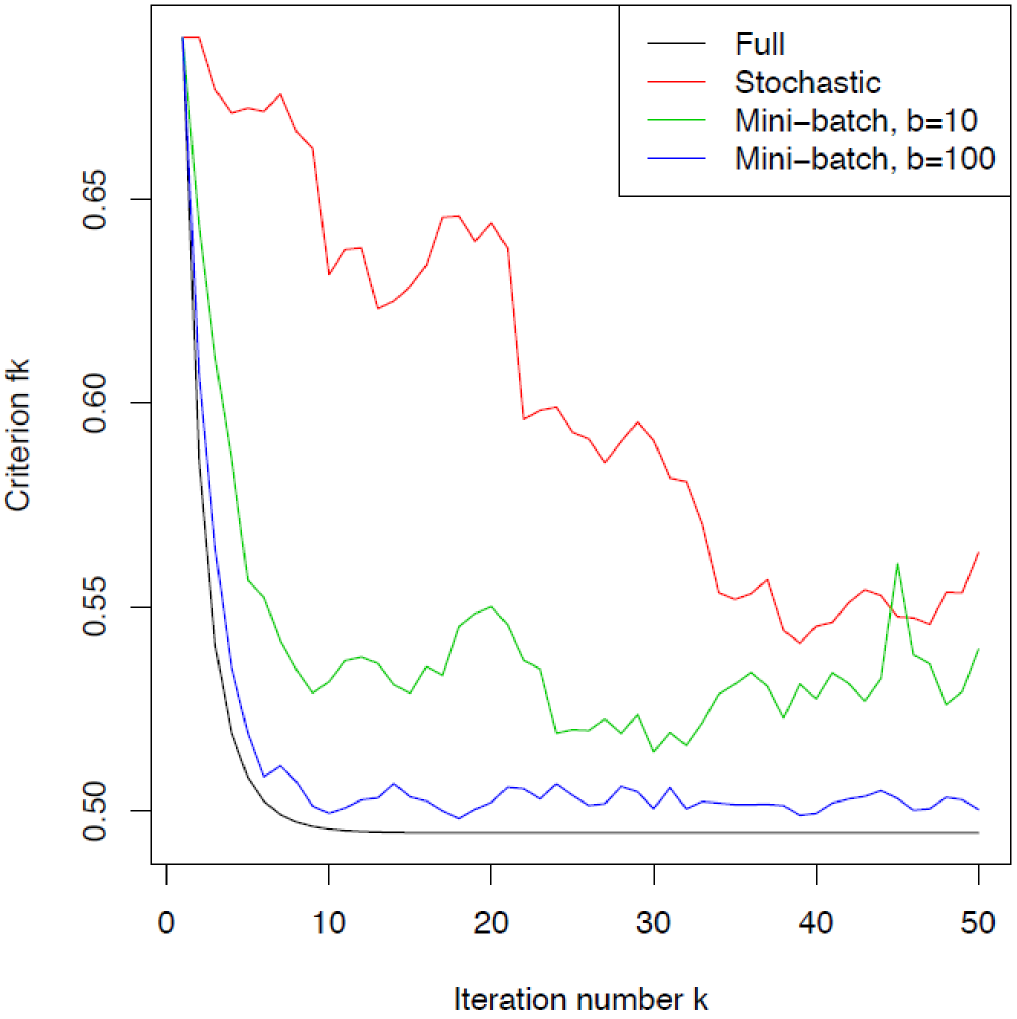
Benefits of stochastic gradient descent

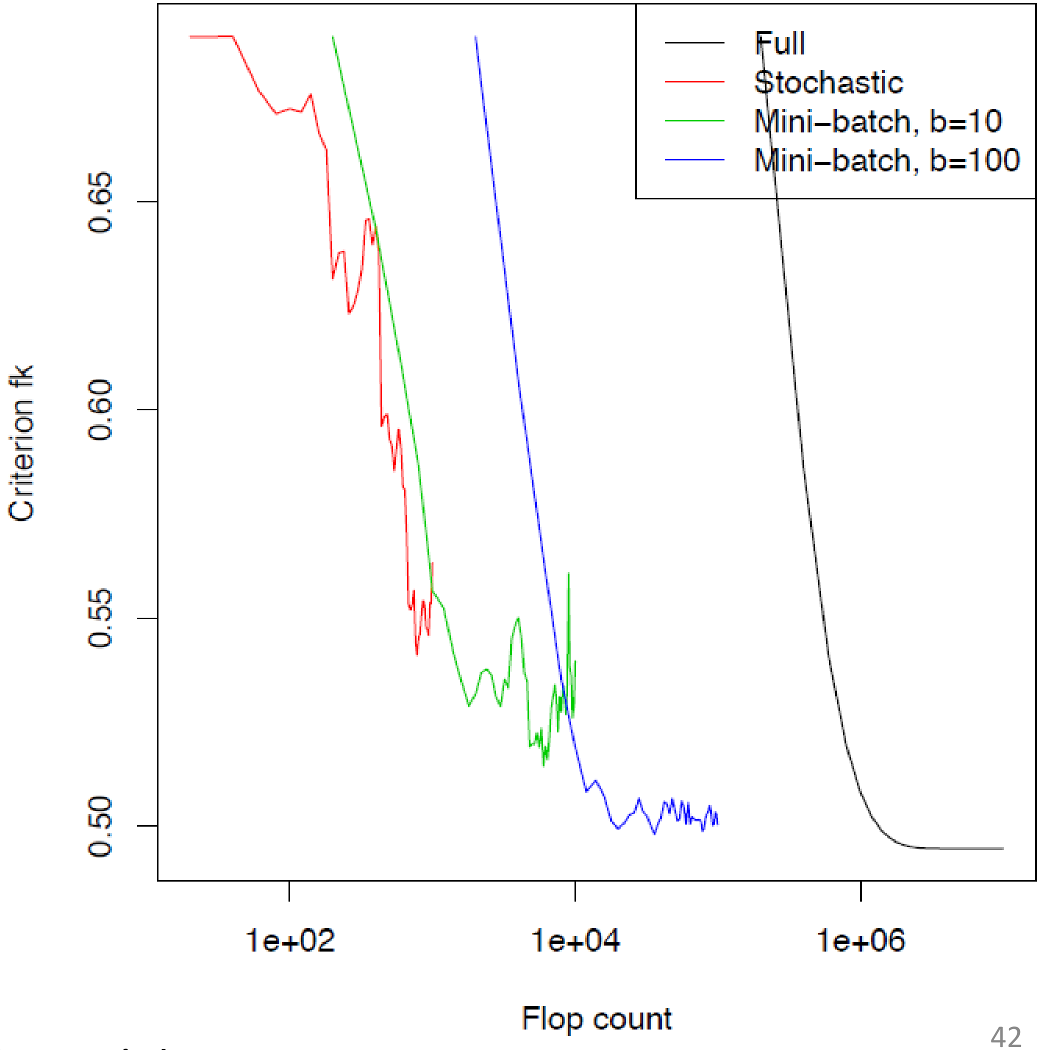


- SGD typically converges much faster than batch update algorithms per accessed data points.
- SGD converges fast at the beginning, but may converge slowly at the end.

Bottou L, Curtis FE, Nocedal J (2018). Optimization methods for large-scale machine learning. *SIAM Review*, 60(2), 223-311.

Stochastic gradient descent for logistic regression





Example from R. Tibsharani's lecture

Quasi-Newton methods

- Gradient descent – uses gradient to determine the next point

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \gamma^{(t)} \nabla f_0(\boldsymbol{x}^{(t)})$$

- Newton's method – uses (expensive) 2nd-order information.

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \left[\nabla^2 f_0(\boldsymbol{x}^{(t)})\right]^{-1} \nabla f_0(\boldsymbol{x}^{(t)})$$

- Quasi-Newton methods approximate Hessian using gradients

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - \gamma^{(t)} \left[H^{(t)}\right]^{-1} \nabla f_0(\boldsymbol{x}^{(t)})$$

where H are iteratively updated using previous gradients

Broygen-Fletcher-Goldfarb-Shanno (BFGS) update.

- BFGS algorithm
  - Let $\boldsymbol{s} = \boldsymbol{x}^{(t)} - \boldsymbol{x}^{(t-1)}$ and $\boldsymbol{y} = \nabla f_0\left(\boldsymbol{x}^{(t)}\right) - \nabla f_0\left(\boldsymbol{x}^{(t-1)}\right)$
  - The BFGS update approximate Hessian using the following rule

$$H^{(t)} = H^{(t-1)} + \frac{\boldsymbol{y}\boldsymbol{y}^T}{\boldsymbol{y}^T\boldsymbol{s}} - \frac{H^{(t-1)}\boldsymbol{s}\boldsymbol{s}^T H^{(t-1)}}{\boldsymbol{s}^T H^{(t-1)}\boldsymbol{s}}$$

- L-BFGS-B algorithm

  Extended version of BFGS with two additional features:
  - Limited memory – compute H more rapidly with less memory.
  - Box constrains – Allow box-like constraints in the optimization problem.

BFGS and L-BFGS-B are implemented in optim()

optim {stats} R Documentation

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      method = c("Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "SANN",
                 "Brent"),
      lower = -Inf, upper = Inf,
      control = list(), hessian = FALSE)

optimHess(par, fn, gr = NULL, ..., control = list())
```

Arguments

`par`	Initial values for the parameters to be optimized over.
`fn`	A function to be minimized (or maximized), with first argument the vector of parameters over which minimization is to take place. It should return a scalar result.
`gr`	A function to return the gradient for the `"BFGS"`, `"CG"` and `"L-BFGS-B"` methods. If it is `NULL`, a finite-difference approximation will be used.

Gradient of logistic objective function

$$f_0(\boldsymbol{\beta}) = -l(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log\left[1 + \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})\right]$$

$$\nabla f_0(\boldsymbol{\beta}) = \sum_{i=1}^{n} \frac{-y_i \boldsymbol{x}_i^T \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})}{1 + \exp(-y_i \boldsymbol{x}_i^T \boldsymbol{\beta})}$$

```
logistic.gradient <- function(b, X, y) {
  tmp <- exp(-y*(X%*%b))
  return( colSums(matrix( -y*tmp/(1+tmp), nrow(X), ncol(X) ) * X)
 )
}
```

Running L-BFGS-B Algorithm

```
optim(c(0,0,0,0,0),
      fn = function(b) { 0-llk2(b, X, y)},
      gr = function(b) { logistic.gradient(b, X, y)},
      method="L-BFGS-B")
```

```
## $par
## [1]  0.35075554  0.09069752 -0.03581004  0.10039737 -0.06488337
##
## $value
## [1] 674.4148
##
## $counts
## function gradient
##        6        6
##
## $convergence
## [1] 0
##
## $message
## [1] "CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH"
```

So far we have learned...

- Single-dimensional optimization
  - Golden section search
  - Brent's method

- Multi-dimensional optimization
  - Nelder-Mead algorithm
  - Coordinate gradient descent
  - Batch (steepest) gradient descent
  - Stochastic gradient descent
  - Quasi-Newton methods : BFGS, L-BFGS-B

These are "generic" algorithms that do not depend on properties of the objective function

Specialized optimization methods

- There are many optimization methods that are specialized for particular subset of optimization problems.

- These methods exploit the intrinsic structure of the problems to more accurately and/or efficiently solve the optimization problems.

- Some specialized optimization methods are still quite general (i.e. applicable to a wide range of similar problems), while some others are tailored only to a particular instance of problem.

Some examples of specialized optimization

- For logistic regression, the standard optimization used is "Iteratively Reweighted Least Squares" (IRWS)

- For LASSO, where we optimizes the following function

$$f(\boldsymbol{\beta}) = \|\boldsymbol{y} - X\boldsymbol{\beta}\|_2 + \lambda\|\boldsymbol{\beta}\|_1 = (\boldsymbol{y} - X\boldsymbol{\beta})^T(\boldsymbol{y} - X\boldsymbol{\beta}) + \lambda\sum_{i=1}^{n}|\beta_i|$$

the "least-angle regression" (LARS) is the algorithm used often.

We won't have time to look into the details of these methods, but there are reasons why these algorithms are well-suited for these particular problems.

Some widely used optimization methods

- Expectation-Maximization (E-M) algorithm
- Simulated annealing
- Linear programming
- Quadratic programming
- Semidefinite programming
- Alternating direction method of multipliers (ADMM)

E-M Algorithm : Overview

- Iterative algorithm for solving MLE problems with missing data

- E-M algorithm is particularly useful when..
  - There are missing (unobserved) data
  - The MLE is analytically intractable if missing data is unobserved
  - The MLE would analytically be tractible if missing data was observed.

- A popular and highly cited (>55,000 times) method.

The basic E-M strategy

- Types of data
  - Complete data $(\boldsymbol{x}, \boldsymbol{z})$: what we would like to have
  - Observed data $\boldsymbol{x}$: individual observations
  - Missing data $\boldsymbol{z}$: hidden/missing values

- The E-M algorithm overview
  1. Initialize the parameter $\boldsymbol{\theta}^{(t)}$
  2. E-step : calculate the distribution of hidden value using current parameter $\boldsymbol{\theta}^{(t)}$
  3. M-step : update the parameter $\boldsymbol{\theta}^{(t+1)}$ to maximize the expected log-likelihood.
  4. Repeat step 2-3 until convergence.

Th Expectation-Maximization algorithm

- E-step

Given $\boldsymbol{\theta}^{(t)}$ and $\boldsymbol{x}$, calculate the following quantity :

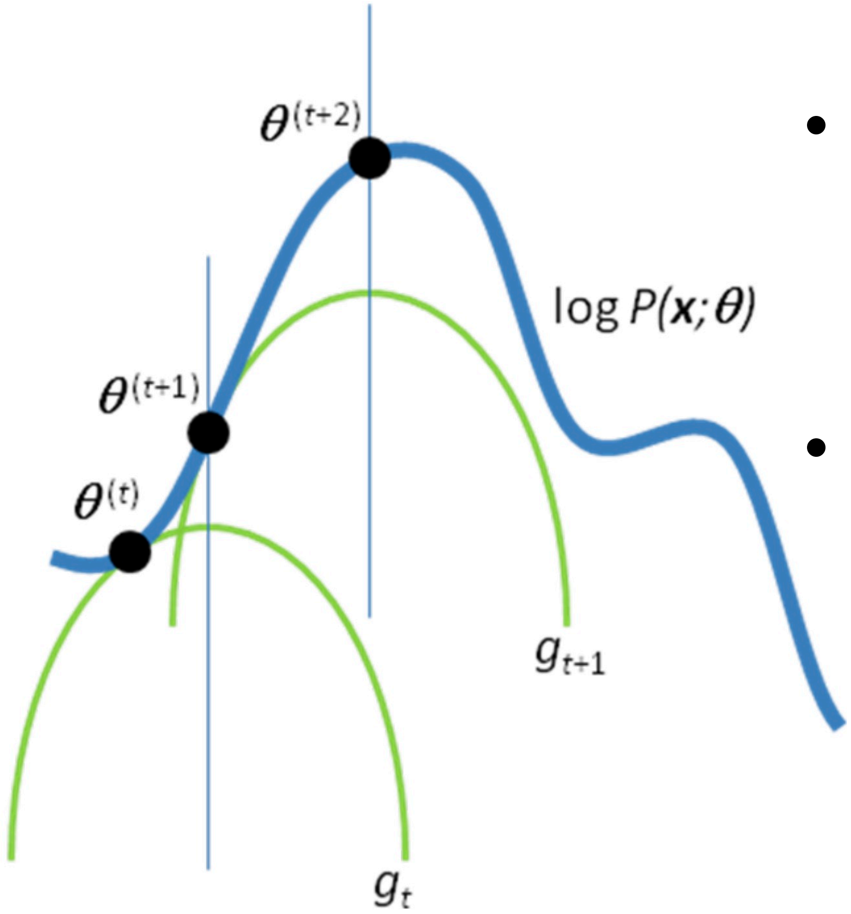
$$w(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\theta}^{(t)}) = \frac{L(\boldsymbol{\theta}^{(t)}|\boldsymbol{x},\boldsymbol{z})}{L(\boldsymbol{\theta}^{(t)}|\boldsymbol{x})} = \frac{f(\boldsymbol{x},\boldsymbol{z}|\boldsymbol{\theta}^{(t)})}{g(\boldsymbol{x}|\boldsymbol{\theta}^{(t)})}$$

- M-step

Find $\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})$ that maximizes the expected log-likelihood

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \mathrm{E}_{\boldsymbol{Z}}\left[\log L(\boldsymbol{\theta}|\boldsymbol{x},\boldsymbol{Z})|\boldsymbol{\theta}^{(t)},\boldsymbol{x}\right] = \int_{\mathcal{Z}} w(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\theta}^{(t)}) \log L(\boldsymbol{\theta}|\boldsymbol{x},\boldsymbol{z}) d\boldsymbol{z}$$

Key property of the E-M algorithm



Do CB and Batzoglou S (2008) *Nat Biotechnol* 26(8):897-89

- The expected log-likelihood function satisfies that

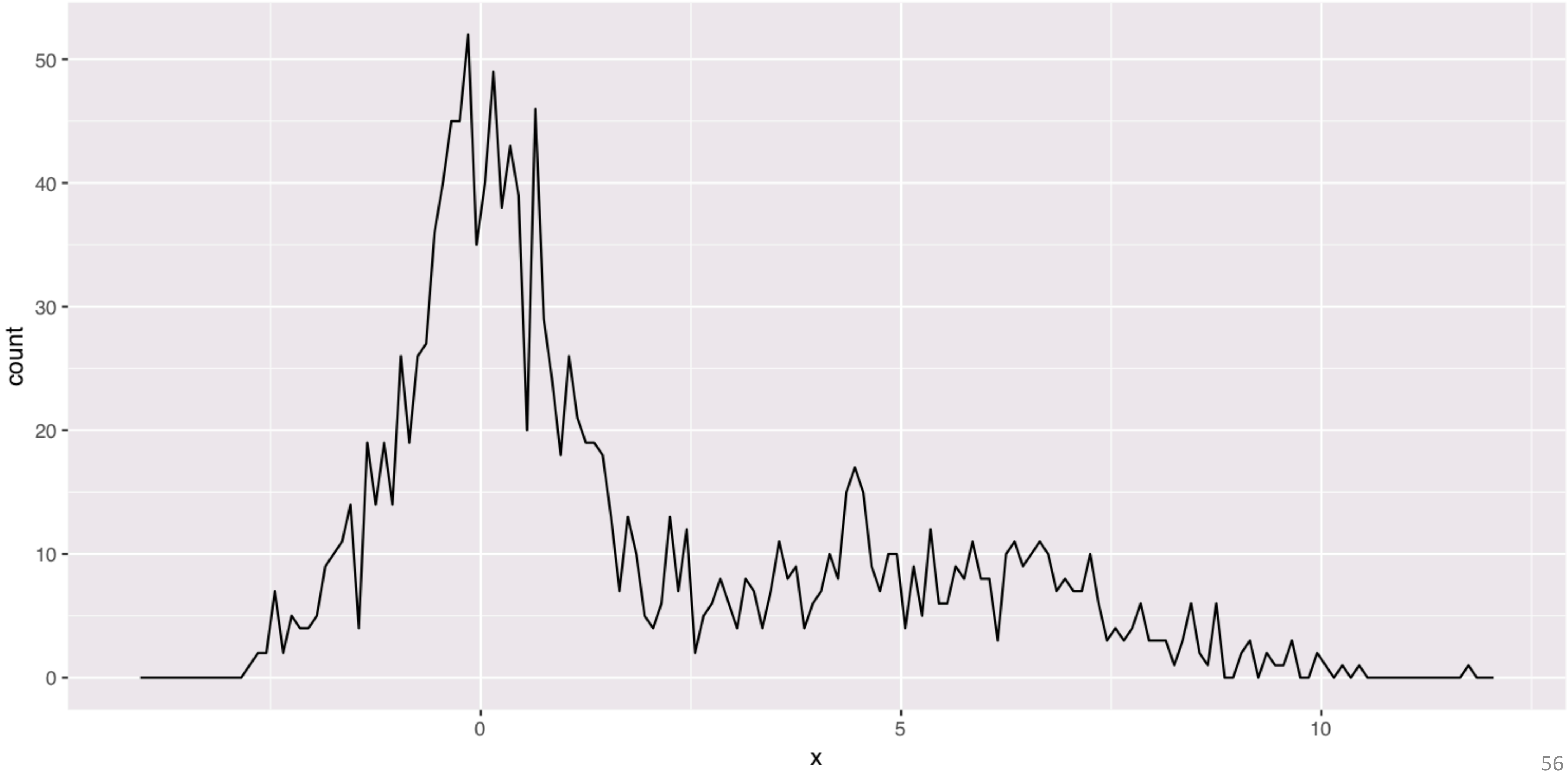
$$g_t(\boldsymbol{\theta}) \leq \log L(\boldsymbol{\theta}|\boldsymbol{x}) \text{ and } g_t(\boldsymbol{\theta}^{(t)}) = \log L(\boldsymbol{\theta}^{(t)}|\boldsymbol{x})$$

- The M-step maximizes the surrogate function, making the likelihood always increase at each iteration.

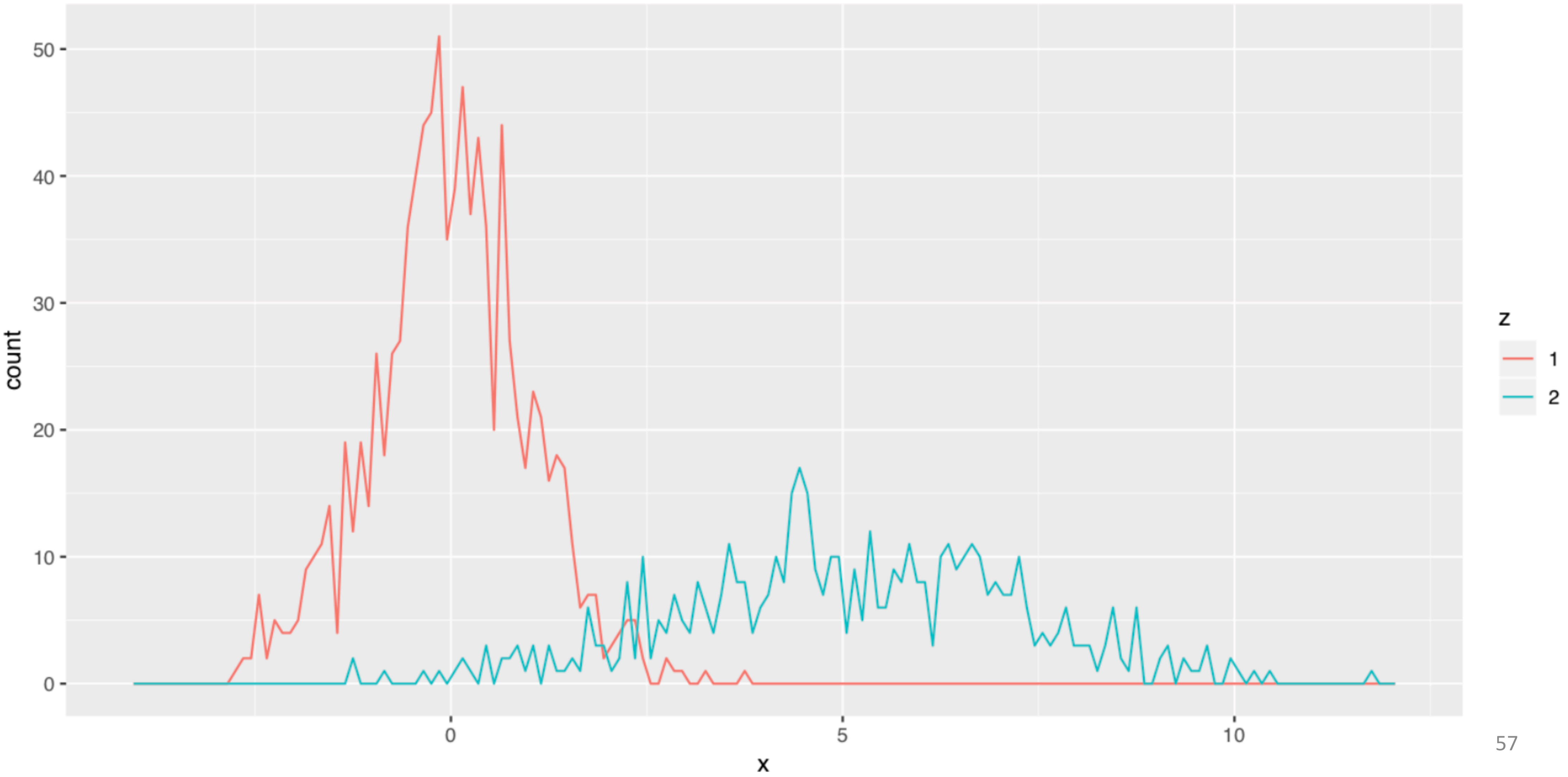
$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} g^{(t)}(\boldsymbol{\theta})$$

$$L(\boldsymbol{\theta}^{(t+1)}|\boldsymbol{x}) \geq L(\boldsymbol{\theta}^{(t)}|\boldsymbol{x})$$

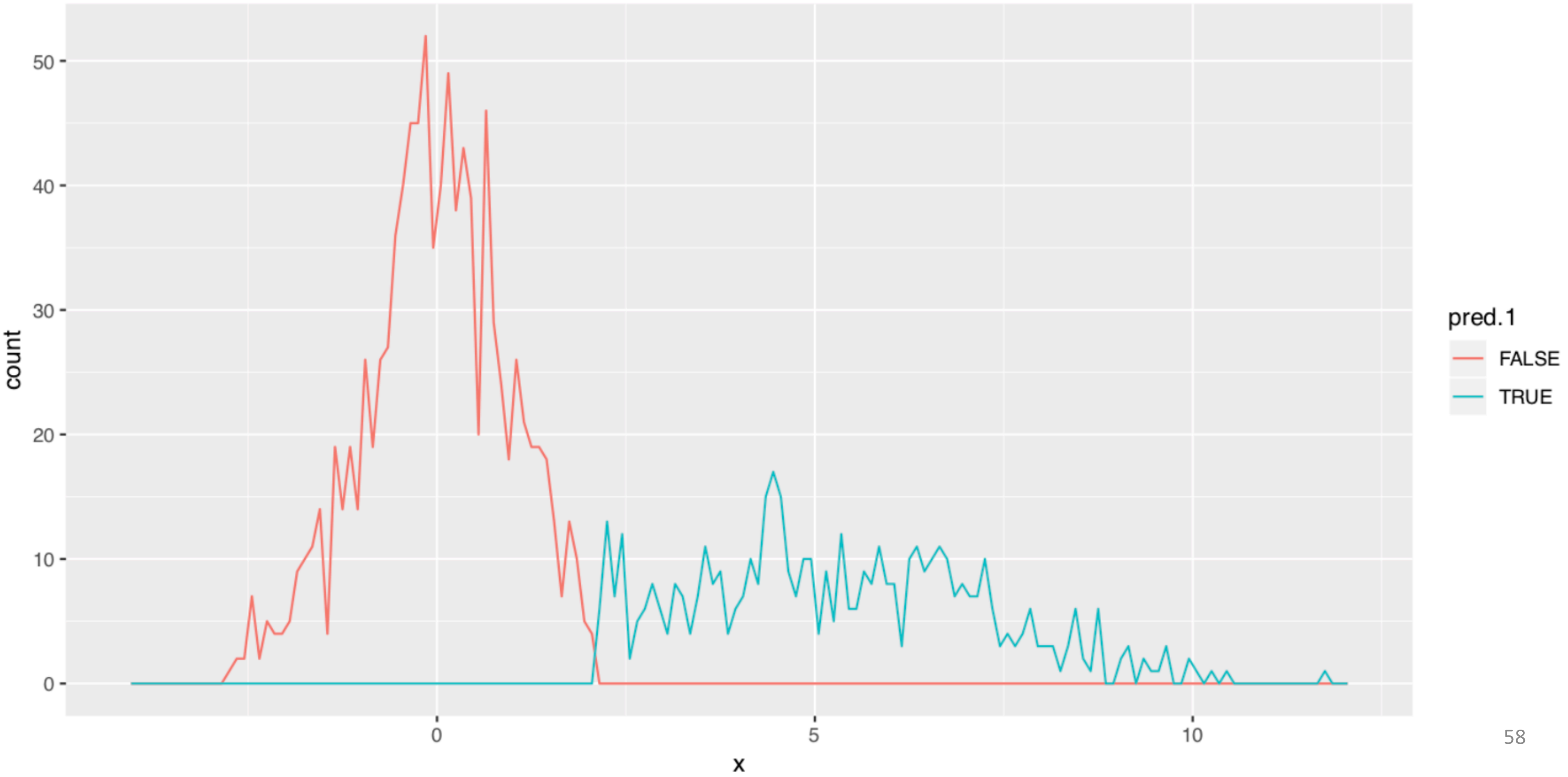
Example – Gaussian mixture model



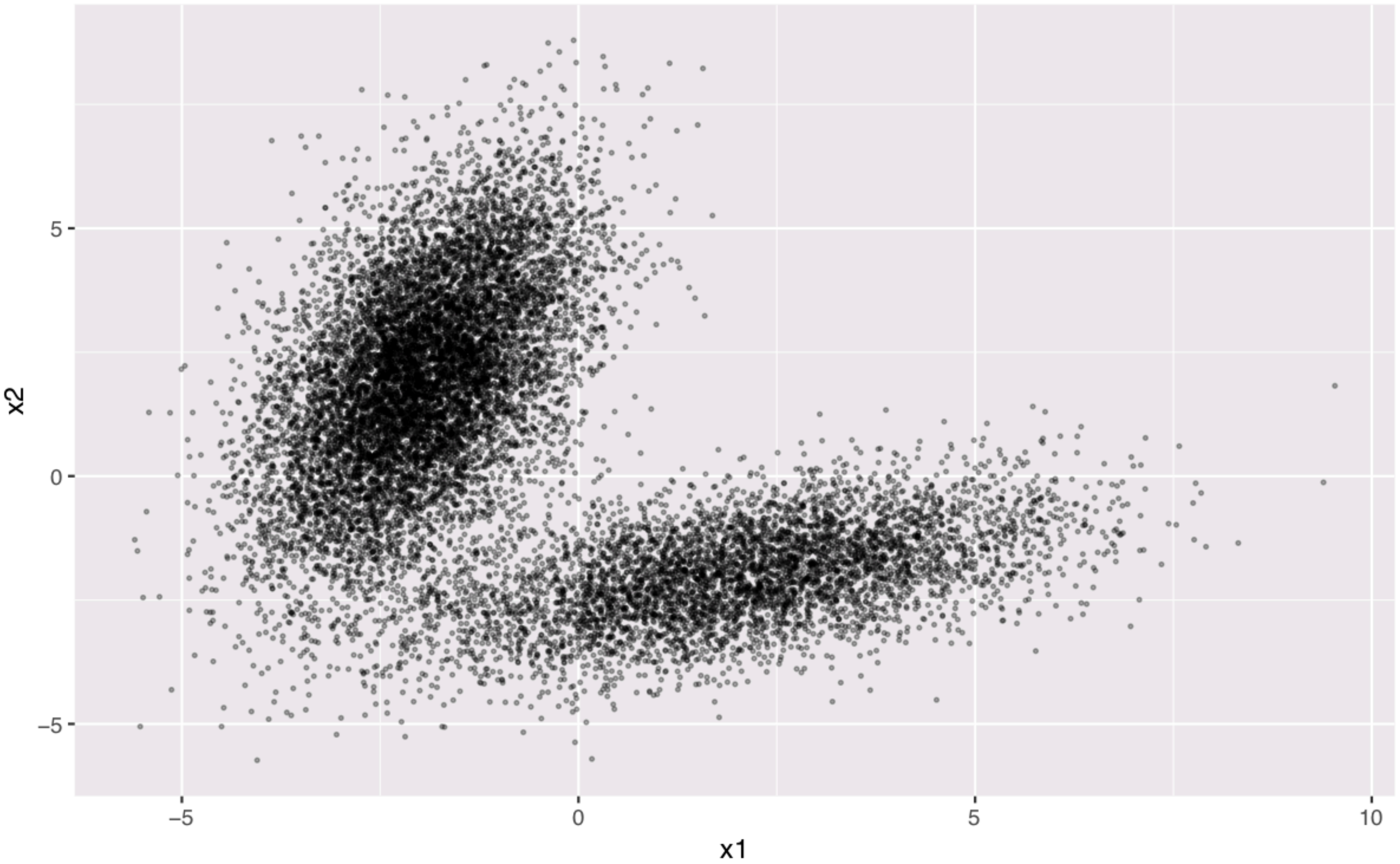
Gaussian mixture model with **true labels**



Labels inferred from the E-M algorithm

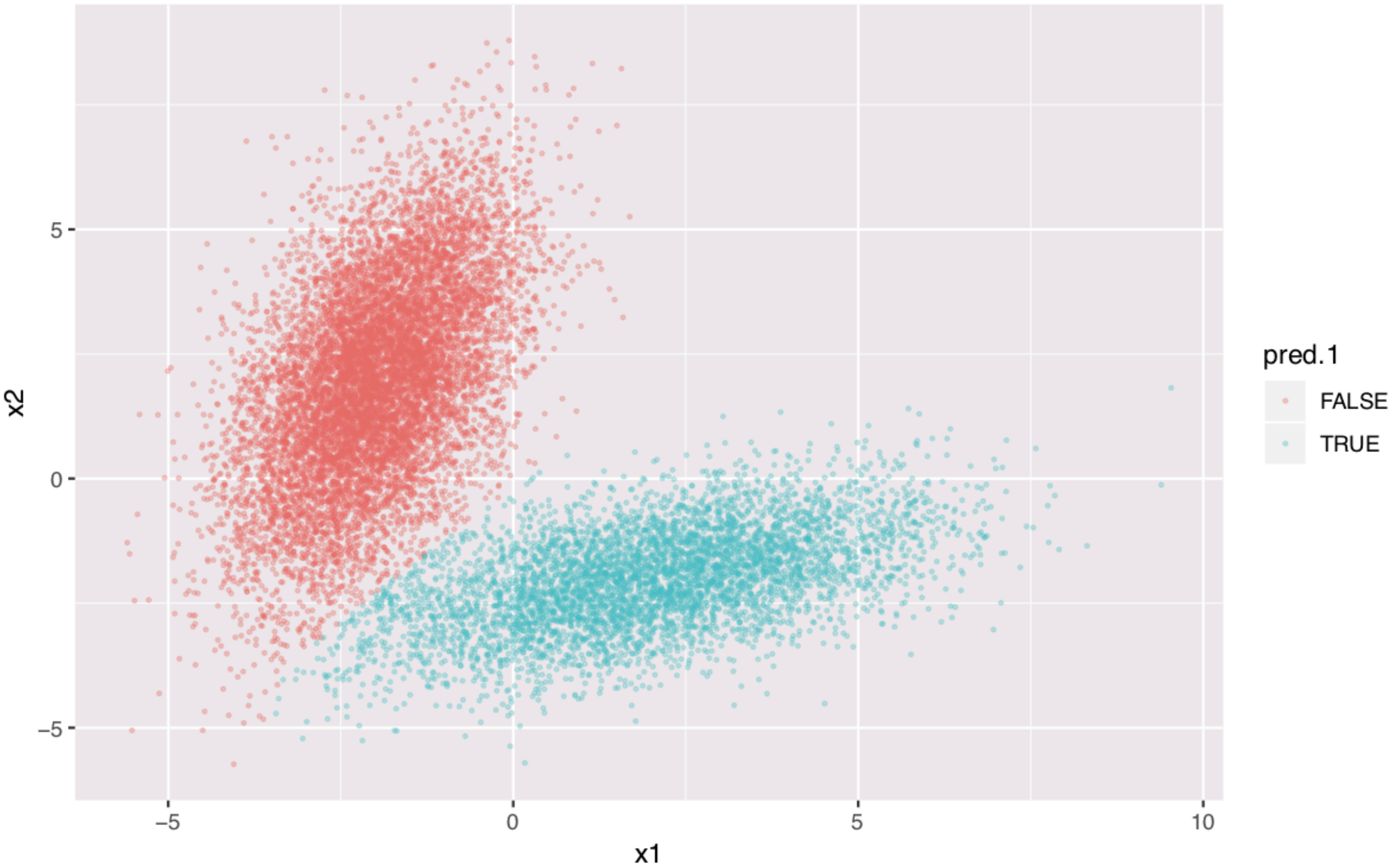


Two dimensional Gaussian mixture



2D Gaussian mixture with true labels

Inferred labels with E-M algorithm



Challenges in hill-climbing methods

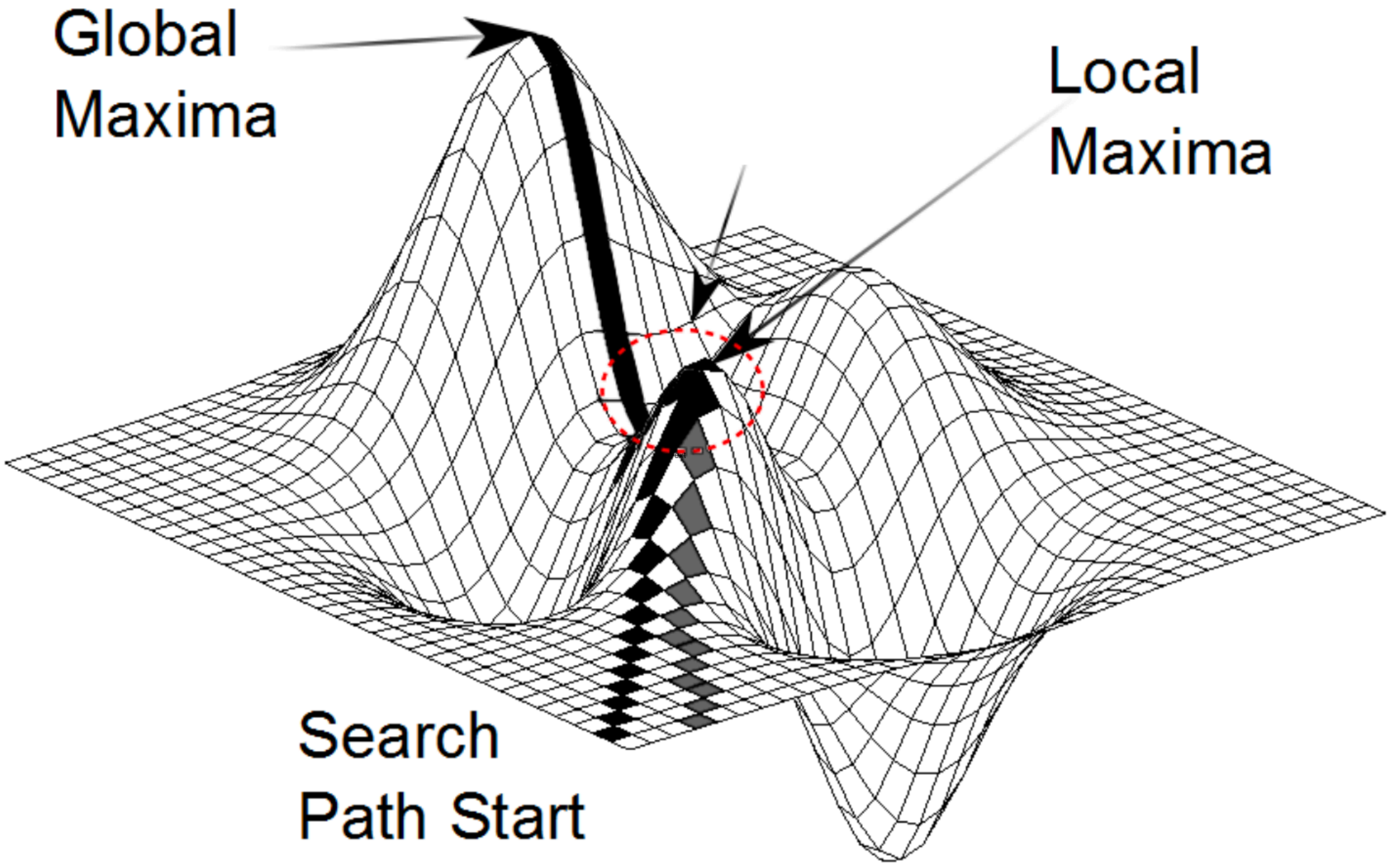


Image : Antal B and Haidu A (2011) *Acta Cybernetica*, 20(5):5-15

Overcoming the challenge : chaotic jump

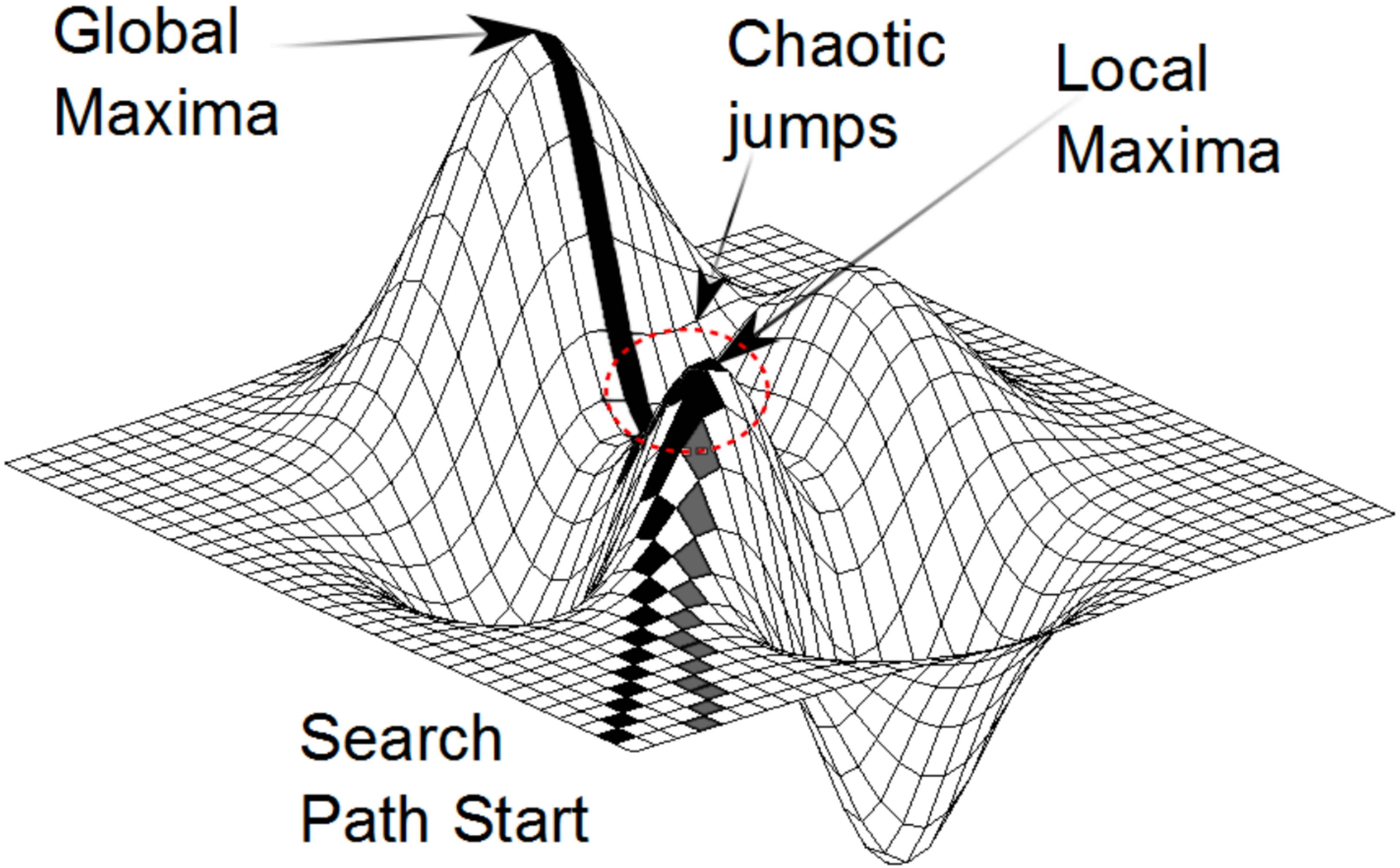
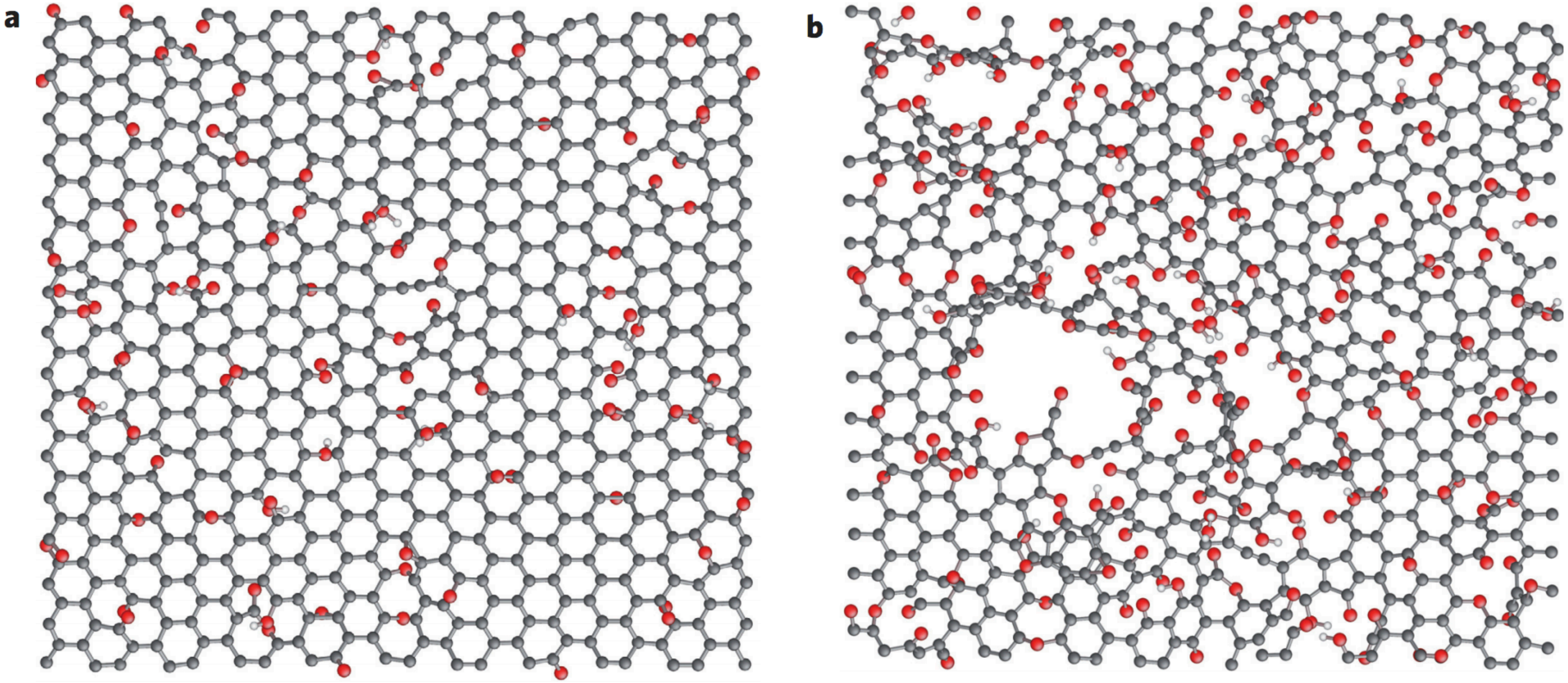


Image : Antal B and Haidu A (2011) *Acta Cybernetica*, 20(5):5-15

Annealing

- Annealing is a manner in which crystals are formed.
- Gradual cooling of liquid can form crystal lattice



Bargi A. et al. (2010) *Nat Chem* 2:581-587

Simulated annealing

- Concept
  - Numerical optimization procedure which aims for global optimization.
  - Use analogy of thermodynamics

- Key idea
  - Incorporates temperature parameter into the optimization procedure
  - At high temperature, explore the parameter space
  - At low temperature, restrict exploration.

Updates in simulated annealing

- Given a temperature, assume a probability proportional to Boltzmann factor

$$P(\boldsymbol{\theta}) \propto \exp\left(-\frac{f_0(\boldsymbol{\theta})}{T}\right)$$

- When updating parameters from $\boldsymbol{\theta}_0$ to $\boldsymbol{\theta}_1$, accept the change probabilistically

$$\min\left(1, \frac{P(\boldsymbol{\theta}_1)}{P(\boldsymbol{\theta}_0)}\right) = \min\left[1, \exp\left(-\frac{f_0(\boldsymbol{\theta}_1) - f_0(\boldsymbol{\theta}_0)}{T}\right)\right]$$

  - New parameter must be chosen based on a random procedure.
  - If the solution was improved, always accept the new parameter.
  - Otherwise, if T is high, the new parameter will be accepted with relatively often.
  - When T is low, the new parameter will be very rarely accepted.

Illustration of simulated annealing procedure

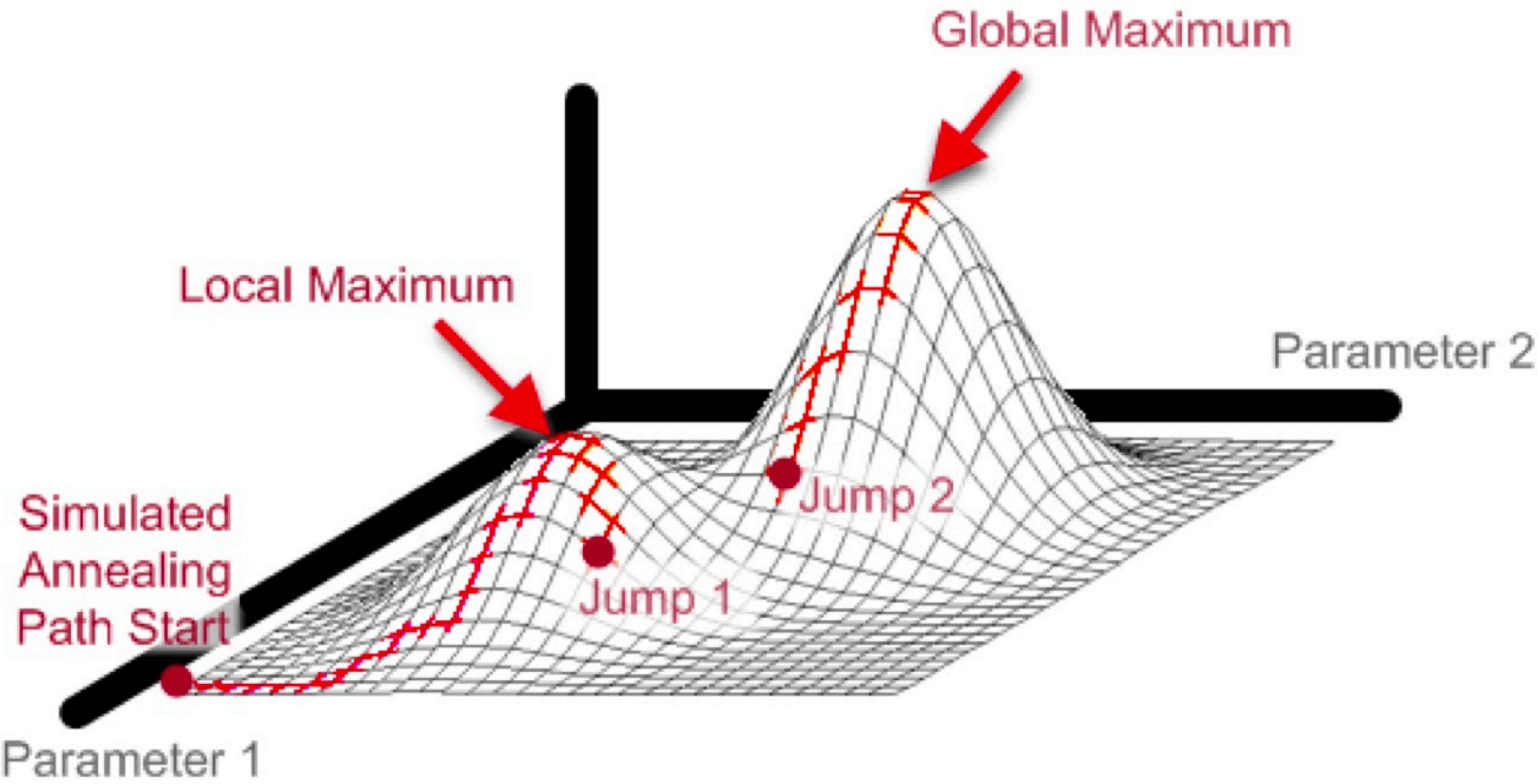
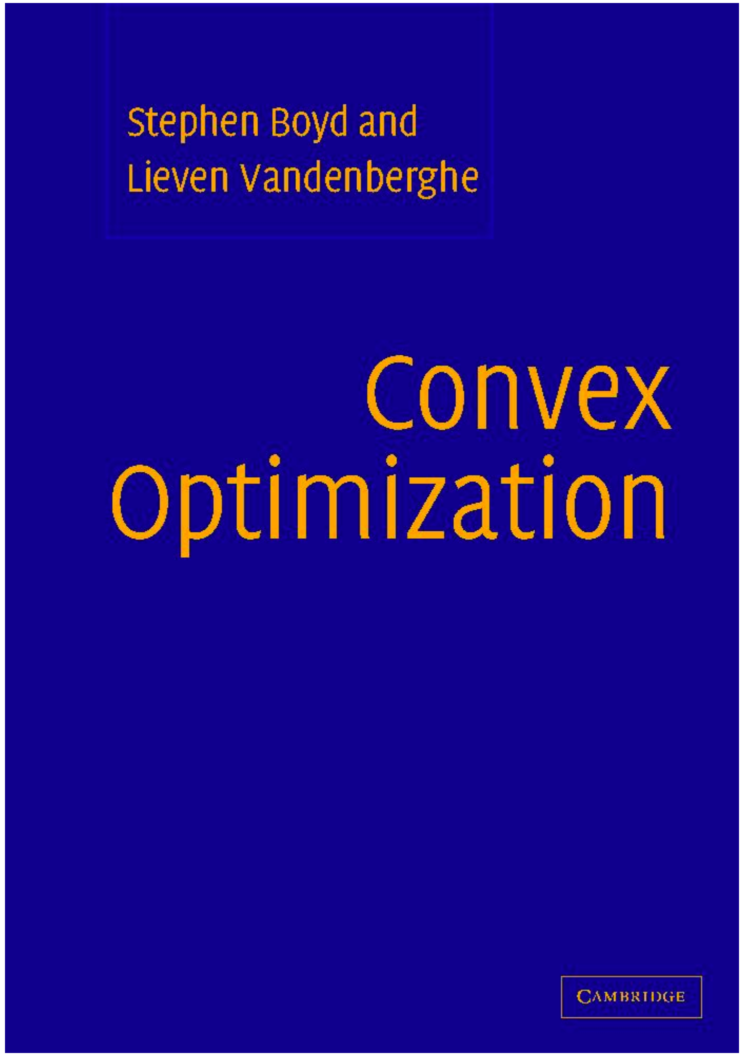


Image by Max Dama

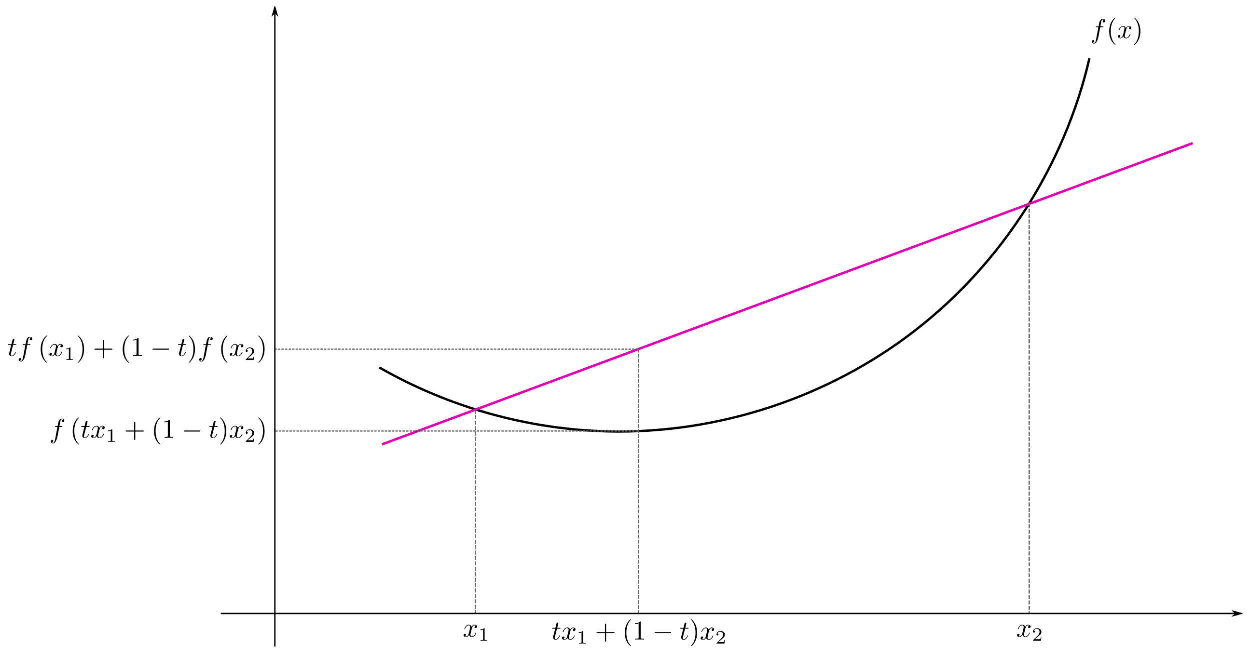
Simulated annealing : highlights

- It is a global optimization method
  - Overcomes disadvantages in hilling-climbing approach
  - Useful to avoid being trapped at local optima for high-dimensional problems
- It is a Markov-chain Monte-Carlo (MCMC) method
  - Randomly updates the the parameter.
  - Probabilistically aceept the new parameter based on Metropolis-Hasting (MH) procedure.
- Useful in solving a variety of optimization problems
  - ..including combinatorial optimization such as the Traveling Salesman Problem
  - implemented in **`optim()`** function in R

Convex optimization



- Convex optimization is a subset of mathematical optimization problem.
- Often there is much easier solution than non-convex optimization problems.



Example : Diet Problem

Doctor's recommendation on diet restriction

- No more than 13,800mg of fat consumption
- At least 600mg, 300mg, 500mg of vitamin X, Y, Z consumptions.

Goal is to come up with most cost-effective diet plan

	Cost /unit	Fat mg/unit	Vitamin X mg/unit	Vitamin Y mg/unit	Vitamin Z mg/unit
Food A	$5.00	800	50	10	150
Food B	$1.00	6,000	3	10	35
Food C	$6.00	1,000	150	75	75
Food D	$3.00	400	100	100	5

Formulating the problem mathematically

- Objective function

$$f_0(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x}, \quad \boldsymbol{c} = [5\ 1\ 6\ 3]^T$$

- Constraint functions

$$\begin{aligned} f_1(\boldsymbol{x}) &= \boldsymbol{a}_1^T \boldsymbol{x} \le b_1 \\ f_2(\boldsymbol{x}) &= \boldsymbol{a}_2^T \boldsymbol{x} \ge b_2 \\ f_3(\boldsymbol{x}) &= \boldsymbol{a}_3^T \boldsymbol{x} \ge b_3 \\ f_4(\boldsymbol{x}) &= \boldsymbol{a}_4^T \boldsymbol{x} \ge b_4 \end{aligned}$$

$$\begin{aligned} \boldsymbol{a}_1 &= [800\ 6000\ 1000\ 400]^T, & \boldsymbol{a}_2 &= [50\ 3\ 150\ 100]^T \\ \boldsymbol{a}_3 &= [10\ 10\ 75\ 100]^T, & \boldsymbol{a}_4 &= [150\ 35\ 75\ 5]^T \\ b_1 &= 13800,\ b_2 = 600, & b_3 &= 300,\ b_4 = 550 \end{aligned}$$

Linear programming (LP)

- Optimization variable

$$\boldsymbol{x} = (x_1, \ldots, x_p) \in \mathbb{R}^p$$

- Objective function : minimize

$$f_0(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x} + d$$

- Constraint functions : subject to

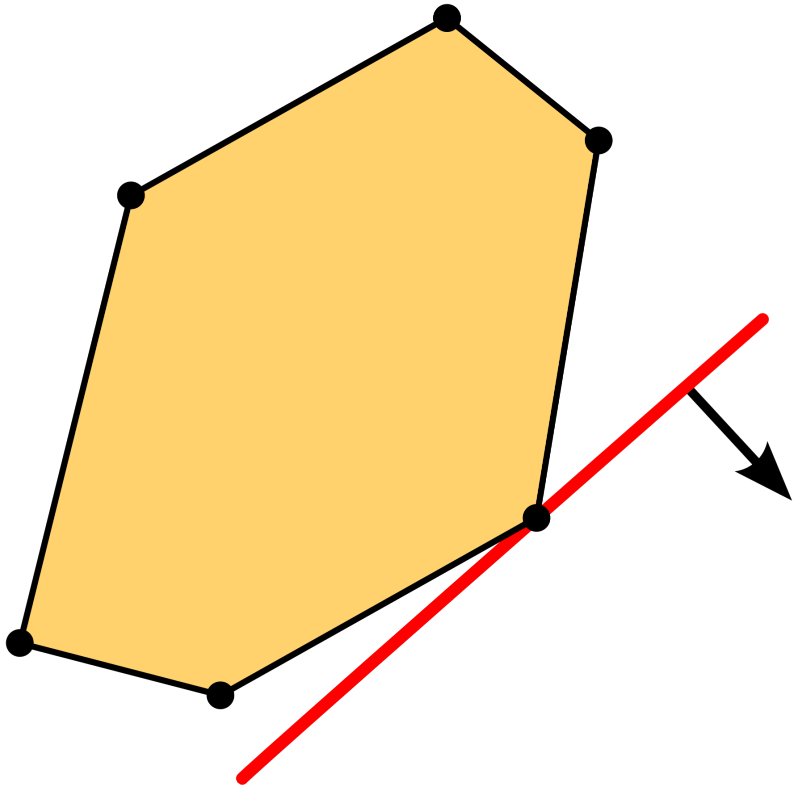
$$\boldsymbol{G}\boldsymbol{x} \preceq \boldsymbol{h}$$

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

$$G \in \mathbb{R}^{m \times p}, A \in \mathbb{R}^{q \times p}$$

Simplex algorithm for LP

- Optimal point occurs in one of the vertices of the simplex
- `boot::simplex()` in R can solve this problem efficiently



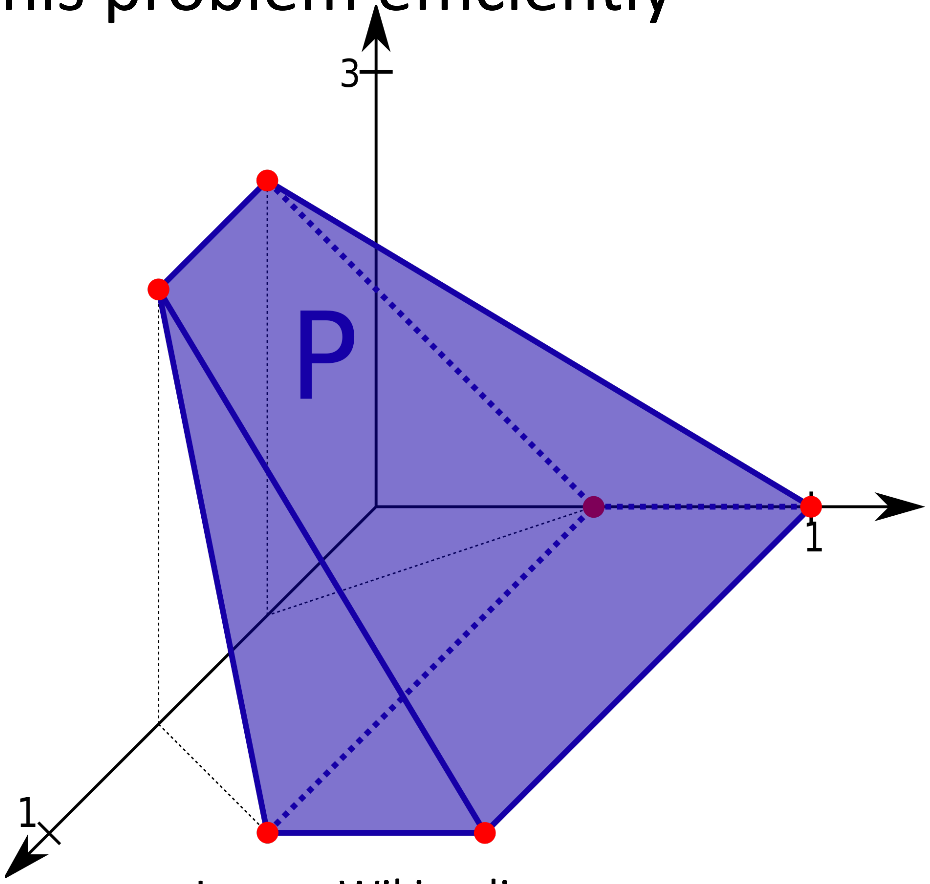


Image: Wikipedia

Quadratic programming (QP)

- Optimization variable

$$\boldsymbol{x} = (x_1, \ldots, x_p) \in \mathbb{R}^p$$

- Objective function : minimize

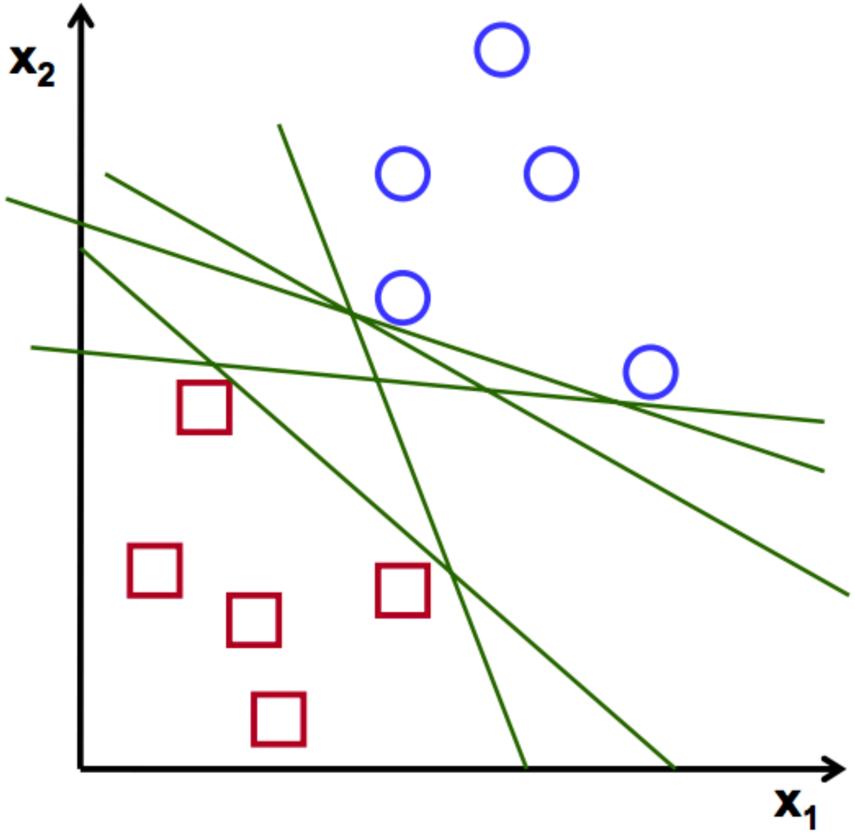
$$f_0(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T P \boldsymbol{x} + \boldsymbol{q}^T \boldsymbol{x} + r$$

- Constraint functions : subject to

$$G\boldsymbol{x} \preceq \boldsymbol{h}$$
$$A\boldsymbol{x} = \boldsymbol{b}$$

$$G \in \mathbb{R}^{m \times p}, A \in \mathbb{R}^{q \times p}$$

Optimally separating hyperplane



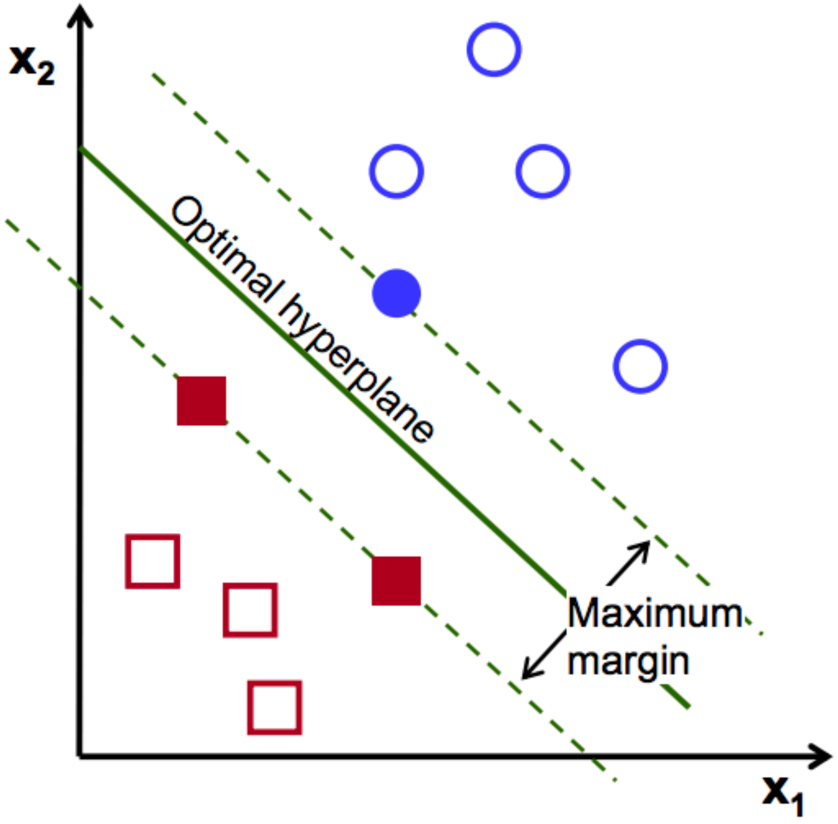
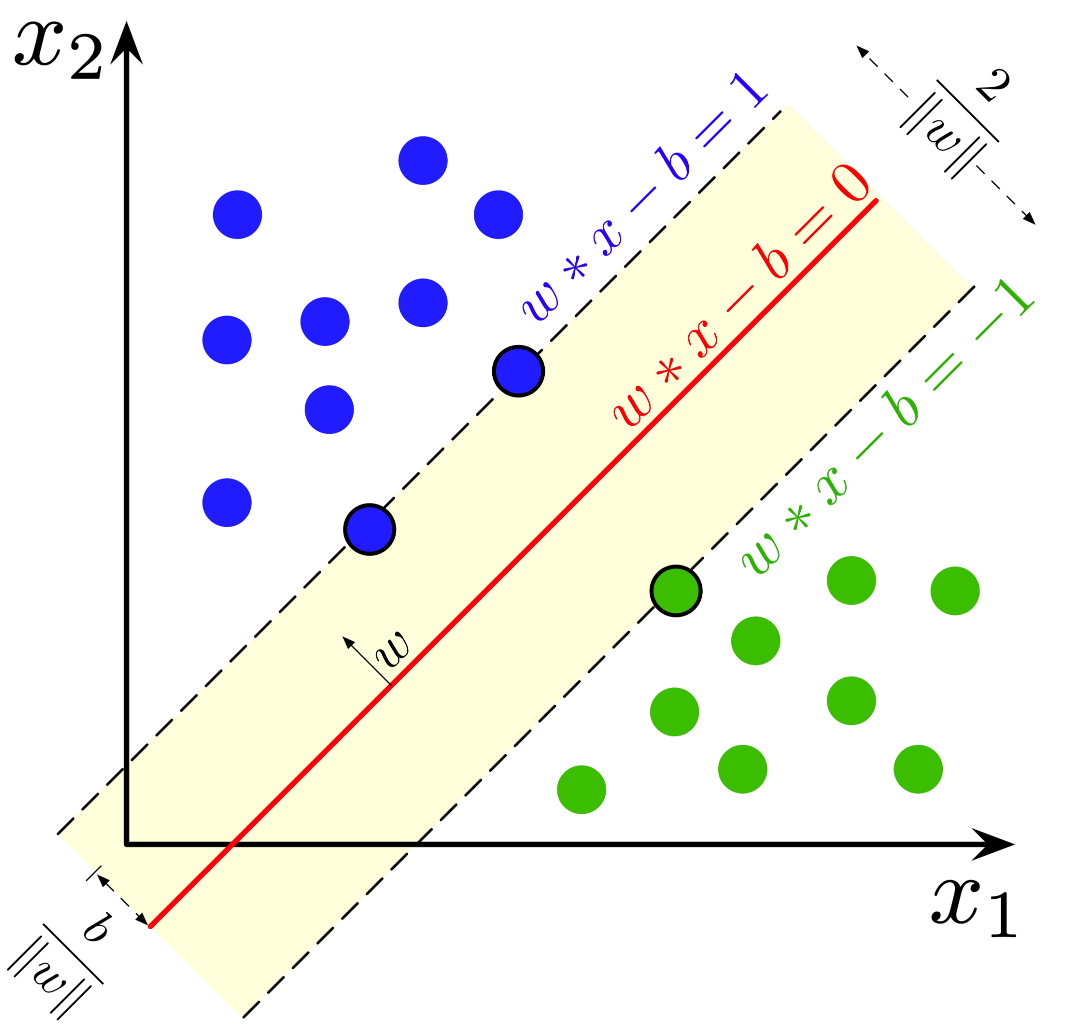


Image: Josephine Sullivan

Maximizing the margin of hyperplane



- Minimize $\frac{1}{2}\|\boldsymbol{w}\|^2 = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w}$
- Subject to $y_i(\boldsymbol{w}^T\boldsymbol{x}_i - b) \geq 1$

  for $i \in \{1, \ldots, n\}$

This is a quadratic programming (QP) problem

Support Vector Machine (SVM)

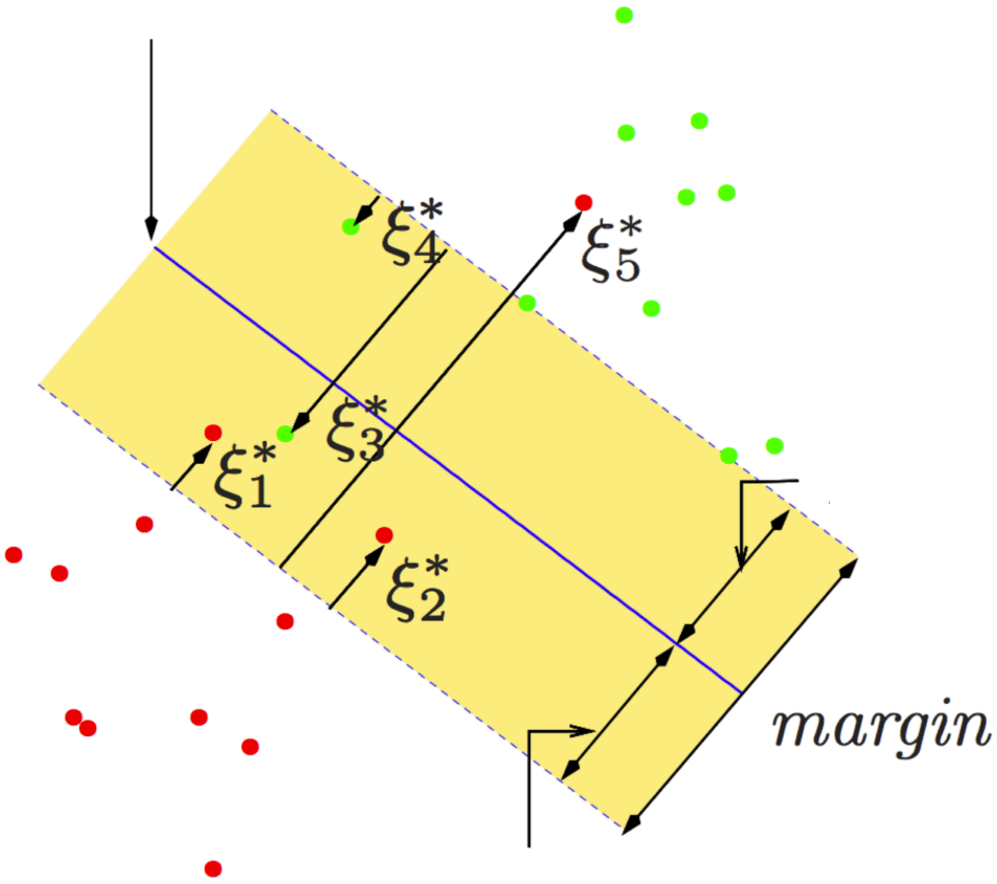


Image: Josephine Sullivan

- To allow non-separable hyperplane, define a hinge loss

$$\xi_i = \max\left(0, 1 - y_i(\boldsymbol{w}^T \boldsymbol{x}_i - b)\right)$$

- Objective function for SVM

Minimize $\frac{1}{2}||\boldsymbol{w}||^2 + C\sum_{i=1}^{n} \xi_i$

where $\xi_i = \max\left(0, 1 - y_i(\boldsymbol{w}^T \boldsymbol{x}_i - b)\right)$

- *This can be represented as a QP, too*
- *Thus, SVM is a QP problem*

Semidefinite programming (SDP)

- Objective function : minimize

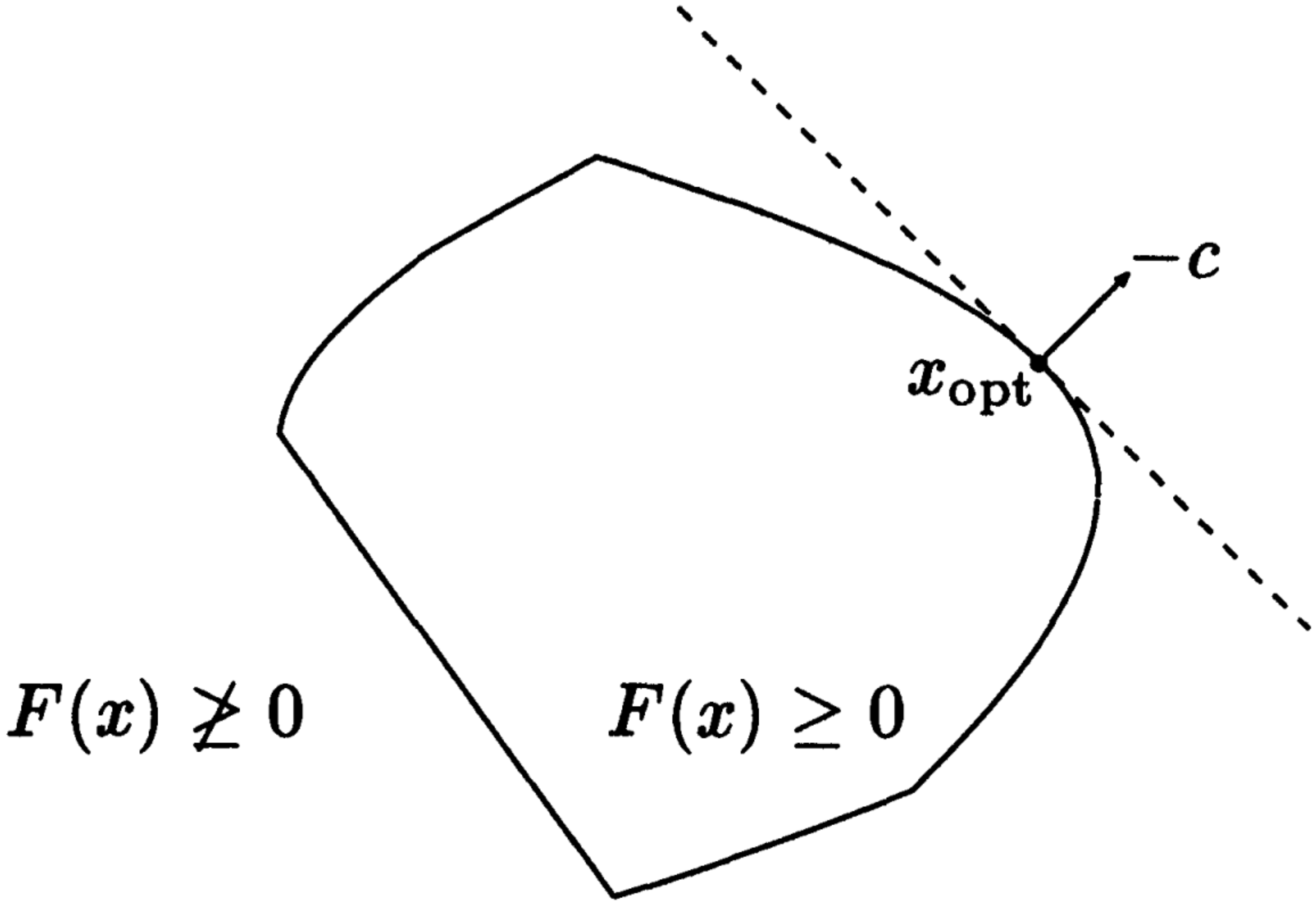
$$f_0(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x}$$

- Constraint functions : subject to

$$F_0 + \sum_{i=1}^{p} x_i F_i \succeq 0$$

$\succeq 0$ represents that the matrix is positive semidefinite (i.e. non-negative eigenvalues)

QP and SDP represent non-linear decision boundary



SDP example from L. Vandenberghe and S. Boyd (1996) *SIAM Review* 38(1): 49-95.

Alternating Direction Method of Multipliers (ADMM)

- Consider convex functions *f* and *g* in the optimization problem.
  - Minimize $f(\boldsymbol{x}) + g(\boldsymbol{z})$
  - Subject to $A\boldsymbol{x} + B\boldsymbol{z} = \boldsymbol{c}$
- The problem assumes two sets of variables that are separable.
- The augmented Lagrangian is defined as

$$\mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{\nu}) = f(\boldsymbol{x}) + g(\boldsymbol{z}) + \boldsymbol{\nu}(A\boldsymbol{x} + B\boldsymbol{z} - \mathbf{c}) + \frac{\rho}{2}\|A\boldsymbol{x} + B\boldsymbol{z} - \mathbf{c}\|_2^2$$

Iterative update steps for ADMM

x-minimization

$$\boldsymbol{x}^{k+1} \leftarrow \arg\min_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{z}^k, \boldsymbol{\nu}^k)$$

z-minimization

$$\boldsymbol{z}^{k+1} \leftarrow \arg\min_{\boldsymbol{z}} \mathcal{L}_\rho(\boldsymbol{x}^{k+1}, \boldsymbol{z}, \boldsymbol{\nu}^k)$$

dual update

$$\boldsymbol{\nu}^{k+1} \leftarrow \boldsymbol{\nu}^k + \rho\left(A\boldsymbol{x}^{k+1} + B\boldsymbol{z}^{k+1} - \boldsymbol{c}\right)$$

Why ADMM?

- Because ADMM is *VERY USEFUL*!

- By separating objective function and constraints into two different functions, ADMM can be used to solve a wide variety of problems.

- Example problems solvable by ADMM
  - LASSO
  - Group LASSO
  - Linear programming
  - Quadratic programming
  - Non-negative matrix factorization (NMF)
  - and more…

Today : Summary

- Generic optimization methods
  - Golden section search
  - Brent’s methods
  - Nelder-Mead algorithm
  - Gradient descent algorithms
  - Quasi-Newton methods (BFGS, L-BFGS-B)
- Specialized optimization methods
  - E-M algorithm
  - Simulated annealing
  - Linear, Quadratic, and Semidefinite Programming
  - ADMM

Important things not covered today

- Markov-Chain Monte Carlo (MCMC) algorithm
- Metropolis-Hasting algorithm
- Gibbs sampler
- Lagrangian
- Lagrangian duality
- Karush-Kuhn-Tucker (KKT) condition
- Dual ascent
- RMSprop
- Adam
- Dynamic programming

These are some keywords you may want to explore later on to learn more about optimization

Optimization: three key questions

1. How can I formulate the problem into an optimization problem?
    - Articulate your problem in mathematical terms.
    - In some cases, you may not even have realized that it is an optimization problem.

2. Do I know how to obtain a solution for the optimization problem?
    - Having an objective function does not automatically solve the problem.
    - Certain optimization problems are much harder than others.

3. Do I know what the time complexity of the method I chose is?
    - If you have big data, time complexity is one of the key factor to consider.
    - The solution should be not only possible but also feasible to obtain.