Optimization Theory for Statistics and Machine Learning

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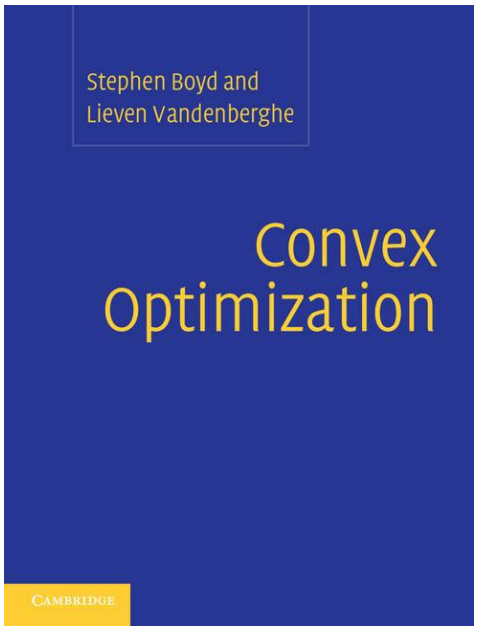
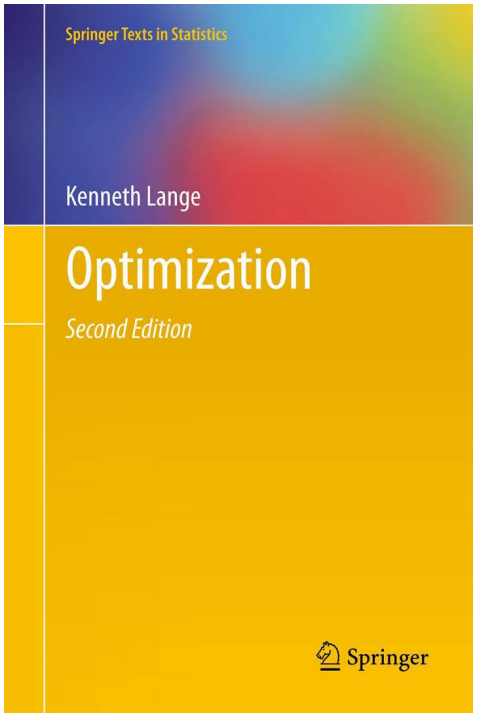
Contents of this course

- Introduce interesting statistical and machine learning problems that can be solved via optimization.
- Present the core concepts of modern optimization theory that are required to solve these modern problems.
- Propose the *MM* algorithm framework as a unifying methodology for constructing optimization algorithms.
- Demonstrate how these algorithms can be implemented within the `R` programming language.
- All course contents can be found at https://github.com/hiendn/CaenOptimization2018.

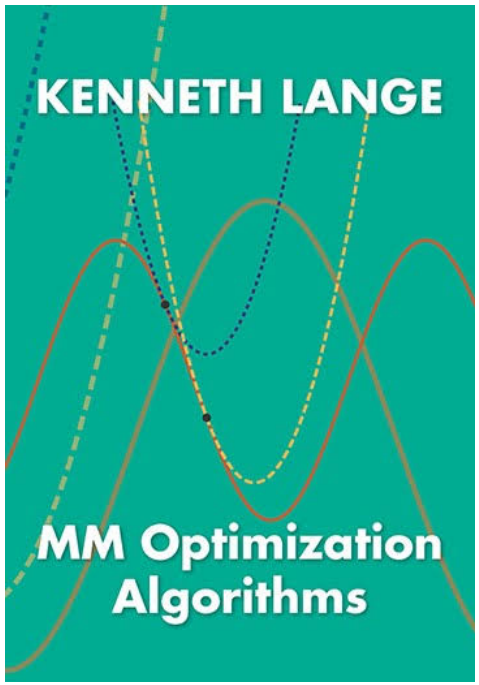
Key readings



(a) Boyd and Vandenberghe, 2004



(b) Lange, 2013



(c) Lange, 2016

Figure 1: The contents of this course can mostly be found in the following books.

What is an optimization problem?

Let $f(\cdot) : \mathbb{T} \to \mathbb{R}$ be an **objective** function of interest, where $\mathbb{T} \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$, and $\mathbb{N}$ and $\mathbb{R}$ denote the **natural** and the **real** numbers, respectively.

We will generally denote a typical element of $\mathbb{T}$ by $\boldsymbol{\theta}$.

The general problem of mathematical **optimization** over real domains $\mathbb{T} \subseteq \mathbb{R}^d$, is find the either the maximum or the minimum values of f over $\mathbb{T}$.

A fair warning

From the famous book of Nesterov (2004), the author gives the following two quotes in the first chapter.

1. Optimization is a very important and promising application theory. It covers almost *all* needs of operations research and numerical analysis.
2. In general, optimization problems are *unsolvable*.

Some examples of optimization problems

Regularized linear regression

Suppose that $y_1, \ldots, y_n \in \mathbb{R}$ are $n \in \mathbb{N}$ observe **responses**, explained by their companion **covariates** $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$.

We wish to determine the coefficients $\alpha \in \mathbb{R}$ and $\boldsymbol{\beta} \in \mathbb{R}^d$, such that the quantity

$$\frac{1}{n} \sum_{i=1}^{n} \left| y_i - \alpha - \boldsymbol{\beta}^\top \boldsymbol{x}_i \right|_p^p + \lambda \sum_{j=1}^{d} |\beta_j|_q^q ,$$

is **minimized**, where $\lambda \in [0, \infty)$ is a **penalty**, $|\theta|_p = |\theta^p|^{1/p}$ for any $\theta \in \mathbb{R}$ and $p, q \in [1, \infty)$. We call $|\theta|_p$ the ℓ_p-norm of the scalar θ. Here, $(\cdot)^\top$ is the matrix transposition operator, and $\boldsymbol{\theta}^\top = (\alpha, \boldsymbol{\beta}^\top) \in \mathbb{R}^{d+1}$, where

$$\boldsymbol{\beta}^\top = (\beta_1, \ldots, \beta_d)^\top .$$

We can, more concisely write the problem as:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^{d+1}} \frac{1}{n} \sum_{i=1}^{n} \left| y_i - \alpha - \boldsymbol{\beta}^\top \boldsymbol{x}_i \right|_p^p + \lambda \sum_{j=1}^{d} |\beta_j|_q^q .$$

An example of the regression problem

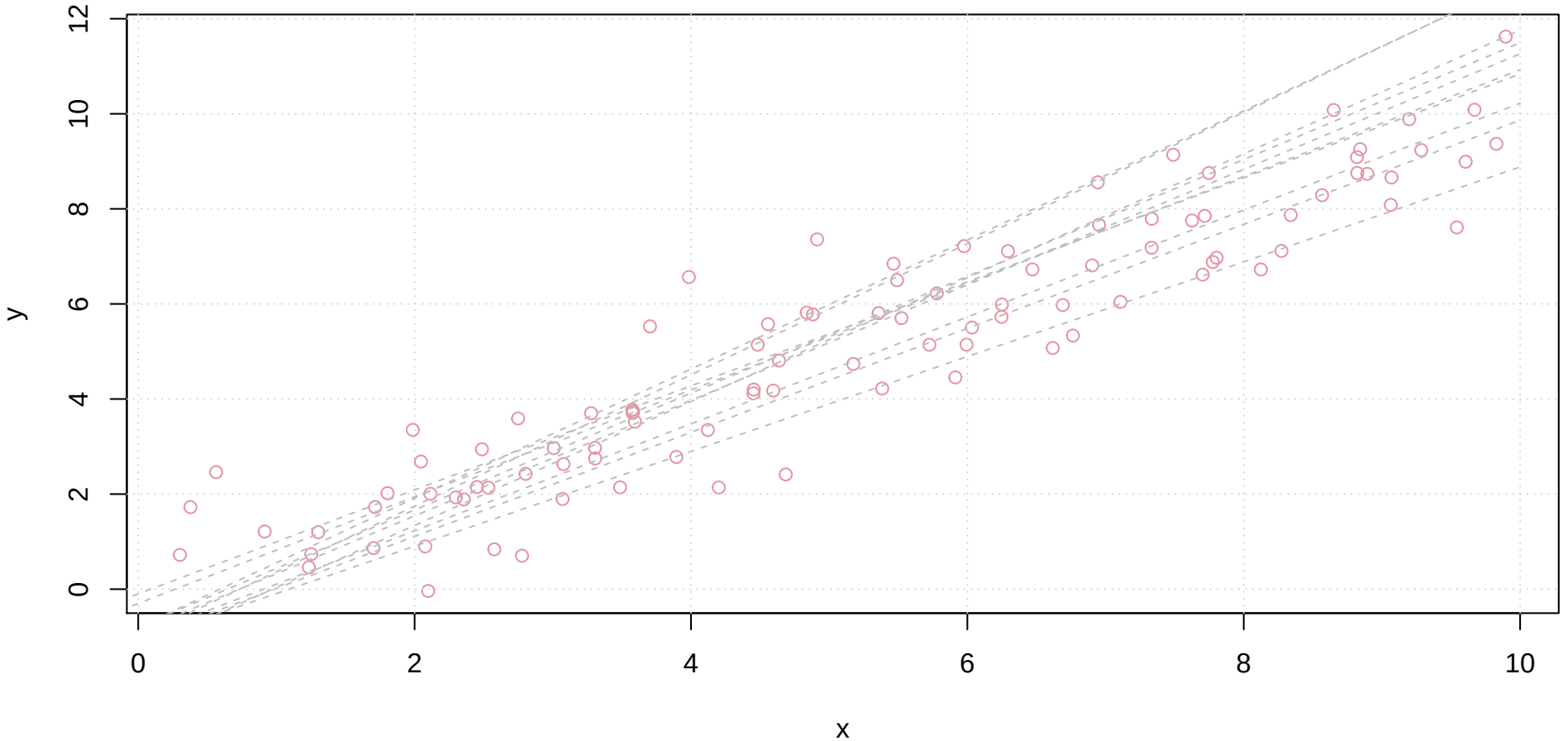


Figure 2: Example of 10 potential linear regression functions when d=1.

Various regularized regression problems

- Ordinary least-squares regression ($p = 2$, $\lambda = 0$).
- Least-absolute deviation regression ($p = 2$, $\lambda = 0$).
- Ridge regression of Hoerl and Kennard (1970) ($p = 2$, $q = 2$, $\lambda > 0$).
- LASSO of Tibshirani (1996) ($p = 2$, $q = 1$, $\lambda > 0$).
- The ℓ_1-LASSO of Wu and Lange (2008) ($p = 1$, $q = 1$, $\lambda > 0$).

Discrimination via optimal seperation hyperplanes

Suppose that $y_1, \ldots, y_n \in \{-1, 1\}$ are n *spin*-binary variables, explained by their companion covariates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$.

We wish to obtain an optimal hyperplane of the form $\alpha + \boldsymbol{\beta}^\top \boldsymbol{x}$, where $\alpha \in \mathbb{R}$, $\boldsymbol{\beta} \in \mathbb{R}^d$, $\boldsymbol{x} \in \mathbb{R}^d$, and $\boldsymbol{\theta}^\top = \left(\alpha, \boldsymbol{\beta}^\top\right)$, such that it minimizes the regularized average **loss**

$$\frac{1}{n} l\left(y_i, \alpha + \boldsymbol{\beta}^\top \boldsymbol{x}_i\right) + \lambda \sum_{j=1}^{d} |\theta_j|_2^2,$$

where $\lambda \in [0, \infty)$, and $l\left(y\alpha + \boldsymbol{\beta}^\top \boldsymbol{x}\right) = \left[y\left(\alpha + \boldsymbol{\beta}^\top \boldsymbol{x}\right) < 0\right]$ is the **classification** loss function.

Here, $[\cdot]$ is the **Iverson bracket** notation which equals 1 if the content is true and 0, otherwise.

Example of hyperplane discrimination functions

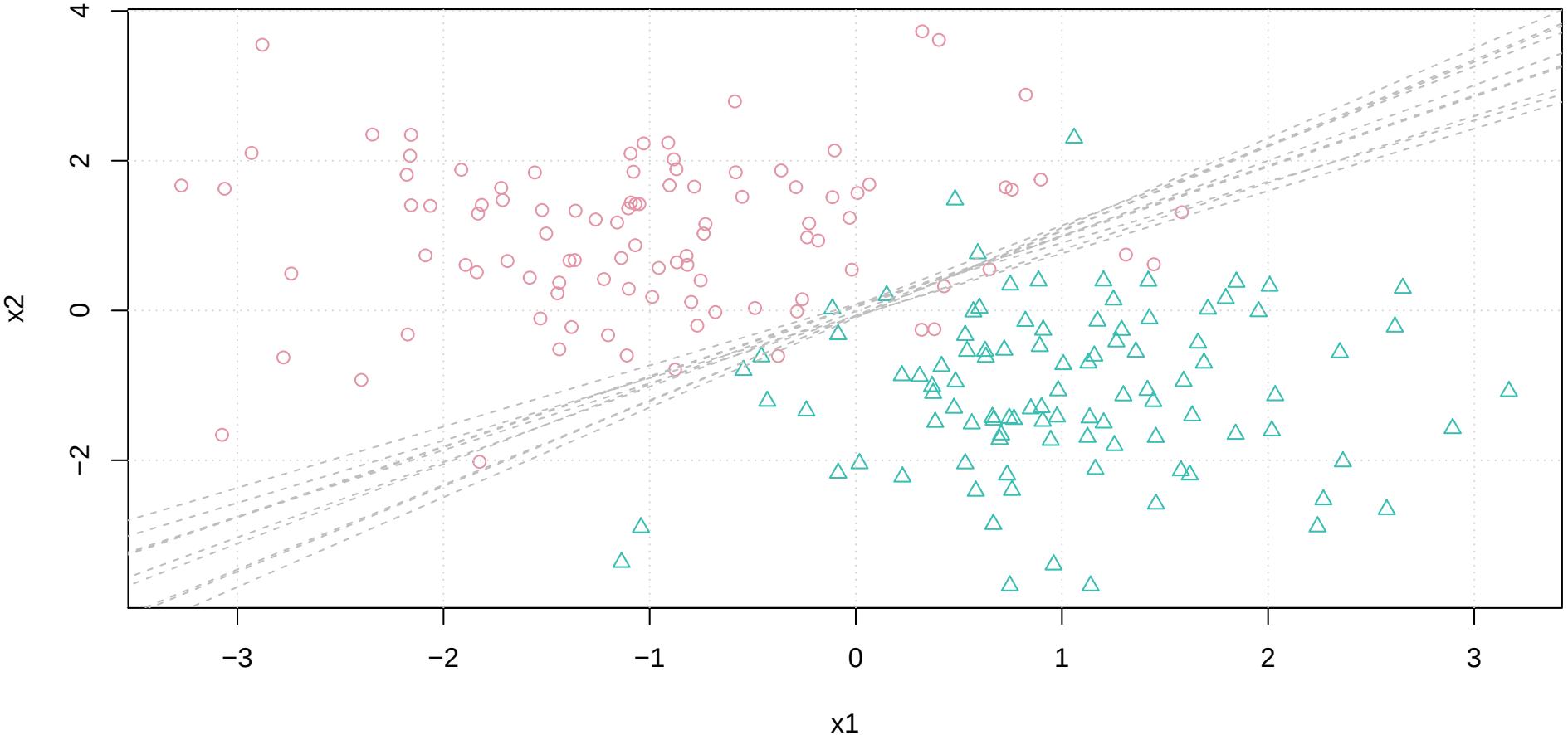


Figure 3: Example of 10 potential discriminant hyperplanes in 2 dimensions.

The support vector machine

The classification loss function

$$l\left(y, \alpha + \beta^\top \boldsymbol{x}\right) = \left[y\left(\alpha + \beta^\top \boldsymbol{x}\right) < 0\right]$$

is *irregular* due to its lack of **convexity** and lack of **differentiability** at the point where $y\left(\alpha + \beta^\top \boldsymbol{x}\right) = 0$, with respect to $\boldsymbol{\theta}$.

In Cortes and Vapnik (1995), the authors proposed a convex approximation of the classification loss function, using the so-called **hinge** loss function

$$l\left(y, \alpha + \beta^\top \boldsymbol{x}\right) = \left[1 - y\left(\alpha + \beta^\top \boldsymbol{x}\right)\right]_+,$$

where $[\cdot]_+ = \max\{0, \cdot\}$.

The resulting optimization problem

$$\min_{\boldsymbol{\theta}=(\alpha,\beta)\in\mathbb{R}^{d+1}} \frac{1}{n}\sum_{i=1}^{n}\left[1 - y_i\left(\alpha + \beta^\top \boldsymbol{x}_i\right)\right]_+ + \lambda\sum_{j=1}^{d}|\beta_j|_2^2,$$

is the original **support vector machine** (SVM) problem.

General SVM problems

- **Logistic regression** is obtained by setting

$$l\left(y, \alpha + \beta^\top \boldsymbol{x}\right) = \log\left[1 + \exp\left(-y\left[\alpha + \beta^\top \boldsymbol{x}\right]\right)\right].$$

- The **least-squares** SVM of Suykens and Vandewalle (1999) is obtained by setting

$$l\left(y, \alpha + \beta^\top \boldsymbol{x}\right) = \left[1 - y\left(\alpha + \beta^\top \boldsymbol{x}\right)\right]^2.$$

- The **truncated-squared** loss SVM of Rosset, Zhu, and Hastie (2004) is obtained by setting

$$l\left(y, \alpha + \beta^\top \boldsymbol{x}\right) = \left[1 - y\left(\alpha + \beta^\top \boldsymbol{x}\right)\right]_+^2.$$

A comparison of loss functions

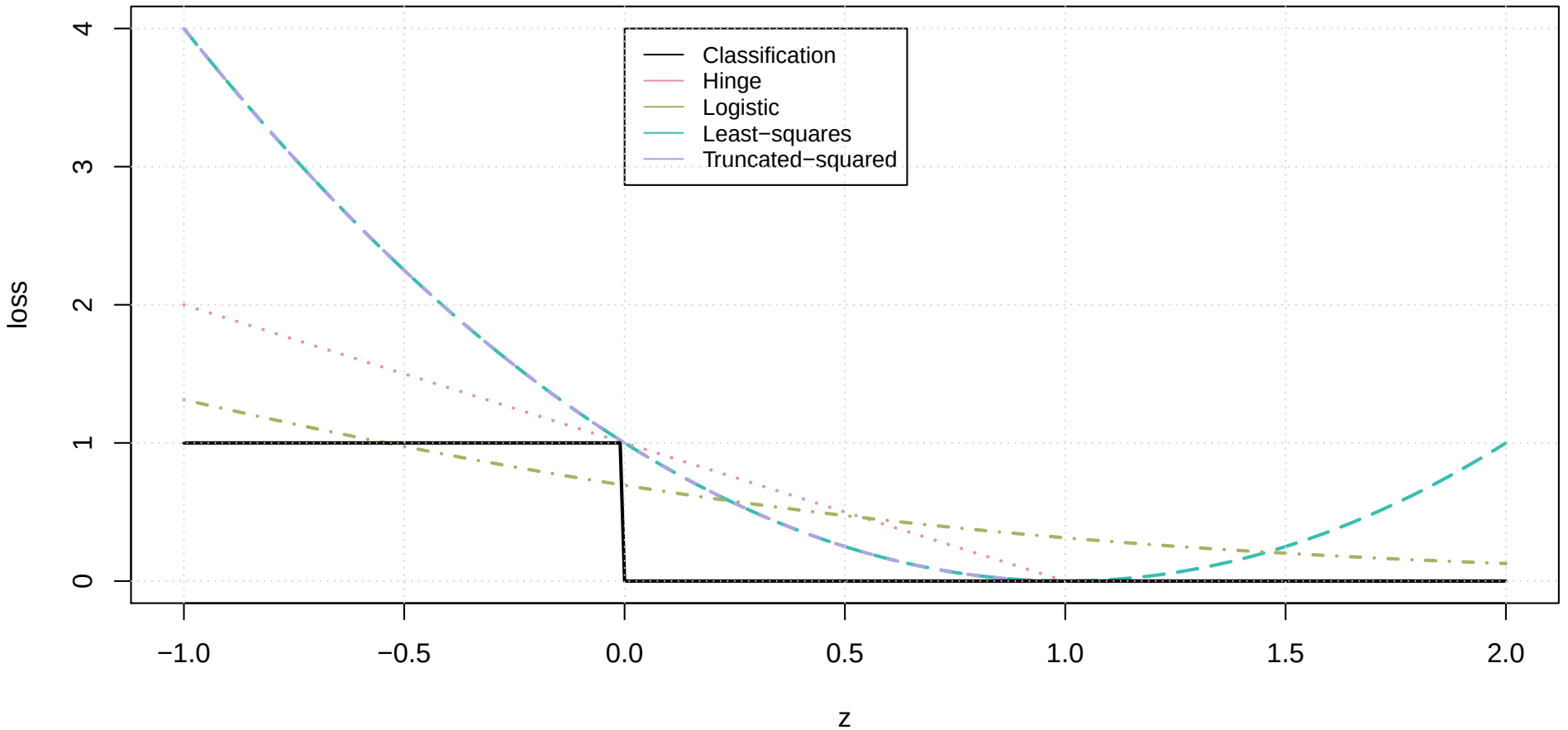


Figure 4: A comparison of SVM loss functions.

Maximum likelihood estimation

Let $\boldsymbol{X} \in \mathbb{X}$ and $\boldsymbol{Y} \in \mathbb{Y}$ be two random variables that share a joint *parametric* **probability density function** (PDF) of known form

$$f(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{\theta}),$$

where $\boldsymbol{\theta} \in \mathbb{T}$ is a **parameter** vector that characterizes the relationship between $\boldsymbol{X}$ and $\boldsymbol{Y}$.

If we observe both $\boldsymbol{X}$ and $\boldsymbol{Y}$ for a **data generating process** (DGP) that can be characterized by the PDF $f(\boldsymbol{x}, \boldsymbol{y}; \boldsymbol{\theta}_0)$, where $\boldsymbol{\theta}_0$ is unknown, then we may estimate it via the method of **maximum likelihood estimation** (MLE), by solving the optimization problem

$$\max_{\boldsymbol{\theta} \in \mathbb{T}} \; \log f\left(\boldsymbol{X}, \boldsymbol{Y}; \boldsymbol{\theta}\right).$$

We say that the value of $\boldsymbol{\theta}$ which solves the problem is the **maximum likelihood estimator** or **estimate** (MLE), and denote it by

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta} \in \mathbb{T}} \; \log f\left(\boldsymbol{X}, \boldsymbol{Y}; \boldsymbol{\theta}\right).$$

Latent variable problems

Suppose that we only observe $\boldsymbol{X}$ and not $\boldsymbol{Y}$, out of the pair. We say that $\boldsymbol{X}$ is **observed** and $\boldsymbol{Y}$ is **hidden** or **latent**.

In such a situation, we can characterize the DGP of what we observe via the *marginal* PDF

$$f\left(\boldsymbol{x};\boldsymbol{\theta}\right) = \int_{\mathbb{Y}} f\left(\boldsymbol{x},\boldsymbol{y};\boldsymbol{\theta}\right) \mathrm{d}\boldsymbol{y}.$$

We can still conduct MLE in order to estimate the value of $\boldsymbol{\theta}_0$ by solving the problem

$$\max_{\boldsymbol{\theta}\in\mathbb{T}} \; \log f\left(\boldsymbol{X};\boldsymbol{\theta}\right),$$

although the task is made more difficult due to the integration over $\boldsymbol{Y}$.

Such problems involving latent variables occur often in statistics, but may still be solvable via the famous *EM* algorithm of Dempster, Laird, and Rubin (1977) if enough structure is known regarding the relationship between $\boldsymbol{X}$ and $\boldsymbol{Y}$.

Examples of latent variable problems

- Elliptical density estimation.
- Factor analysis.
- Finite mixture models.
- Hidden Markov modeling.
- Linear mixed-effects modeling.
- Multiple missing data imputation.
- Non-negative matrix factorization.
- Probabilistic principal component analysis.
- Skew density estimation.

Finite mixture models

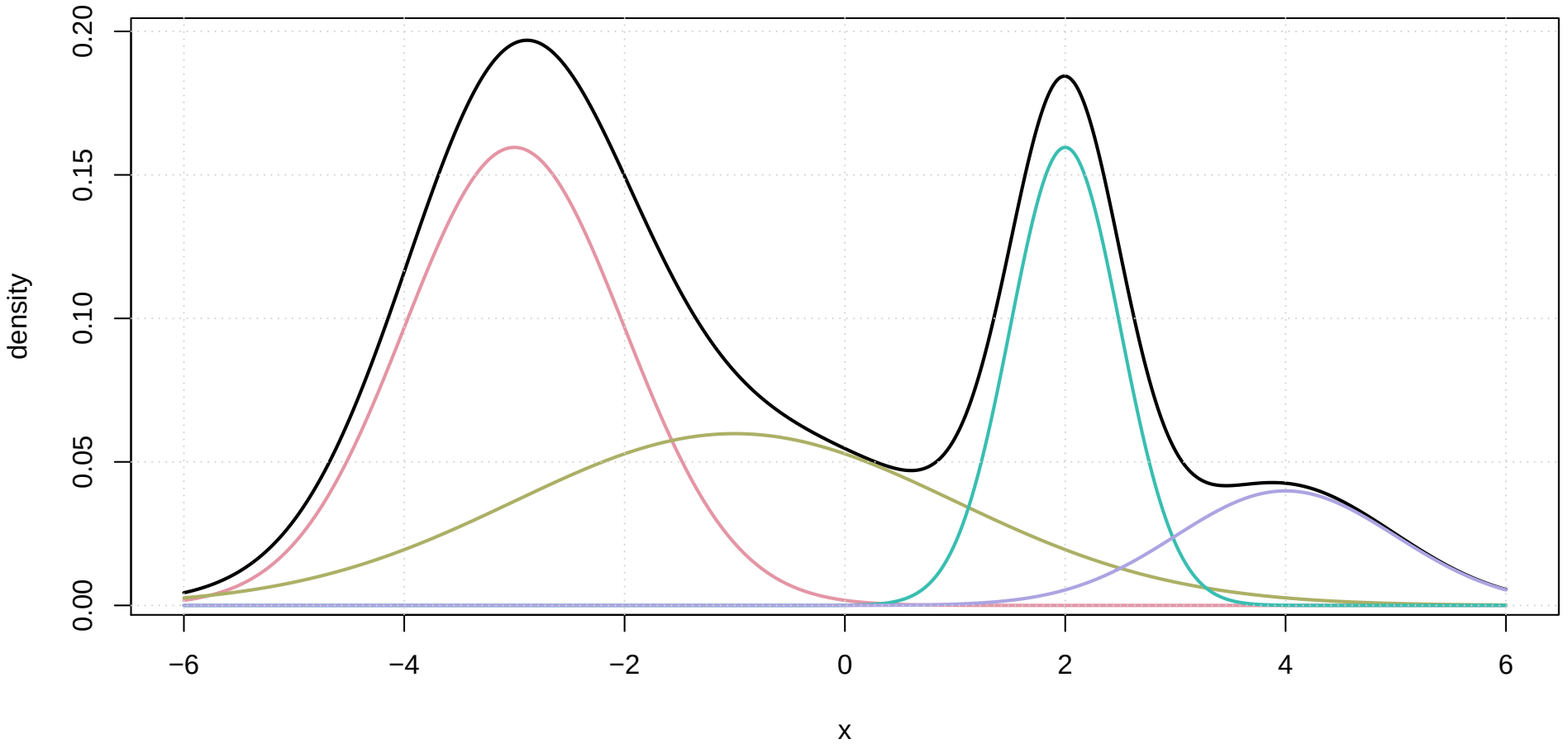


Figure 5: A 4-component mixture of normal PDFs.

Fundamental definitions and results

Global maxima and minima

We say that a point $\boldsymbol{\theta}^*$ in the **domain** or **support** (i.e. $\mathbb{T}$) of $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is a **global maximizer** if

$$f(\boldsymbol{\theta}^*) \geq f(\boldsymbol{\theta}),$$

for all $\boldsymbol{\theta} \in \mathbb{T}$. We call the value $f(\boldsymbol{\theta}^*)$ the **global maximum**.

If

$$f(\boldsymbol{\theta}^*) > f(\boldsymbol{\theta}),$$

for all $\boldsymbol{\theta} \neq \boldsymbol{\theta}^*$, then we say that $\boldsymbol{\theta}^*$ is a **strict** global maximizer. Notice that by definition, a strict global maximizer must be *unique*, if it exists.

The definition of **global minimizer**, **global minimum**, and **strict** global minimizer can be obtained by reversing the inequalities.

The Euclidean norm

For any $p \in [1, \infty)$, denote the ℓ_p vector norm by

$$\|\boldsymbol{\theta}\|_p = \left(\sum_{j=1}^{d} |\theta_j|^p \right)^{1/p},$$

where $\boldsymbol{\theta}^\top = (\theta_1, \ldots, \theta_d) \in \mathbb{R}^d$.

Setting $p = 2$, we obtain the ℓ_2 norm $\|\cdot\|_2$, which is generally referred to as the **Euclidean norm**.

The Euclidean metric

We say that a function

$$\Delta(\cdot,\cdot) : \mathbb{R}^d \times \mathbb{R}^d \to [0,\infty)$$

is a **metric** if, for all $\boldsymbol{\psi}, \boldsymbol{\theta}, \boldsymbol{\upsilon} \in \mathbb{R}^d$, it satisfies the conditions:

1. $\Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon}) \geq 0$.
2. $\Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon}) = 0$ if and only if $\boldsymbol{\theta} = \boldsymbol{\upsilon}$.
3. $\Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon}) = \Delta(\boldsymbol{\upsilon}, \boldsymbol{\theta})$.
4. $\Delta(\boldsymbol{\psi}, \boldsymbol{\upsilon}) \leq \Delta(\boldsymbol{\psi}, \boldsymbol{\theta}) + \Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon})$.

It can ben shown that setting

$$\Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon}) = \|\boldsymbol{\theta} - \boldsymbol{\upsilon}\|_p$$

yields a metric for any $p \in [0,\infty)$. Again, in the case where $p = 2$, we obtain the **Euclidean metric**

$$\Delta(\boldsymbol{\theta}, \boldsymbol{\upsilon}) = \|\boldsymbol{\theta} - \boldsymbol{\upsilon}\|_2 .$$

Local maxima and minima

If we equip our real space $\mathbb{T} \subseteq \mathbb{R}^d$ with the Euclidean norm, then we obtain the **Euclidean metric space**, which equips our space with *topological* properties that can be used to characterize functional behavior.

We now define a **local maximizer** as a point $\boldsymbol{\theta}^* \in \mathbb{T}$, such that there exists some $\epsilon > 0$ for which $f(\boldsymbol{\theta}^*) \geq f(\boldsymbol{\theta})$, for all

$$\boldsymbol{\theta} \in B_\epsilon(\boldsymbol{\theta}^*) = \left\{ \boldsymbol{\theta} \in \mathbb{R}^d : \|\boldsymbol{\theta} - \boldsymbol{\theta}^*\|_2 < \epsilon \right\}.$$

The value $f(\boldsymbol{\theta}^*)$ is then defined as a **local maximum**. Here, we say that the $B_\epsilon(\boldsymbol{\theta}^*)$ is the ϵ (Euclidean) **ball** of $\boldsymbol{\theta}^*$.

We can define a **strict** local maximizer by replacing the $\geq$ symbol by a $>$ symbol.

Furthermore, we can define **local minimizer**, **local minimum**, and **strict** local minimizer by reversing the inequalities.

A bit of set theory

We say that a point $\boldsymbol{\theta}^* \in \mathbb{R}^d$ is a **limit point** of $\mathbb{T}$ if for every ball $N_\epsilon(\boldsymbol{\theta}^*)$, there exists a

$$\boldsymbol{\theta} \in \mathbb{T} \cup N_\epsilon(\boldsymbol{\theta}^*).$$

We can now define a **closed** set in a *real metric space* as a set that contains all of its limit points. Furthermore, we can say that a set $\mathbb{T}$ is **open** if its *complement* $\mathbb{R}^d \backslash \mathbb{T}$ is closed.

We say that a set $\mathbb{T} \subset \mathbb{R}^d$ is **bounded** if there exists a finite ϵ and some $\boldsymbol{\theta} \in \mathbb{R}^d$, such that

$$\mathbb{T} \cup N_\epsilon(\boldsymbol{\theta}) = \mathbb{T}.$$

By the famous *Heine-Borel theorem*, every closed and bounded set in the Euclidean metric space is **compact**.

A first existence theorem

When $\mathbb{T} \subset \mathbb{R}$, the **extreme value theorem** in calculus states that if $\mathbb{T} = [a, b]$, where $-\infty < a < b < \infty$, and if $f(\cdot) : [a, b] \to \mathbb{R}$ is *continuous*, then there exists $c, d \in [a, b]$, such that

$$f(c) \leq f(\theta) \leq f(d),$$

for all $\theta \in [a, b]$.

The famous *Weierstrass optimimality theorem* generalizes the extreme value theorem, and states that if $\mathbb{T} \subset \mathbb{R}^d$ is compact and if $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is continuous, then there exists $\boldsymbol{\psi}, \boldsymbol{\upsilon} \in \mathbb{T}$, such that

$$f(\boldsymbol{\psi}) \leq f(\boldsymbol{\theta}) \leq f(\boldsymbol{\upsilon}),$$

for all $\theta \in \mathbb{T}$.

Thus, if $\mathbb{T}$ is compact and f is continuous, then there exists at least one global minimizer and one global maximizer of f.

Differentiable functions

Suppose now that f is **continuously differentiable** on any open subset of $\mathbb{T}$. That is, if $\mathbb{S} \subseteq \mathbb{T}$ is open, then the **gradient**

$$\left[\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*)\right]^\top = \left(\frac{\partial f}{\partial \theta_1}(\boldsymbol{\theta}^*), \ldots, \frac{\partial f}{\partial \theta_d}(\boldsymbol{\theta}^*)\right)$$

exists for every $\boldsymbol{\theta}^* \in \mathbb{S}$.

We say that $\boldsymbol{\theta}^* \in \mathbb{T}$ is a **stationary point** of f, if it satisfies the equation

$$\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*) = \mathbf{0},$$

where $\mathbf{0}$ is a matrix or vector of zeros of appropriate dimensionality.

If $\boldsymbol{\theta}^*$ is a local maximum or local minimum of f in some open subset of $\mathbb{T}$, and if f is continuously differentiable, then it is *necessary* that $\boldsymbol{\theta}^*$ is also a stationary point of f.

A second existence theorem

In a metric space, we say that $\boldsymbol{\theta}^*$ is an **interior point** of a set $\mathbb{T}$ if there exists an $\epsilon > 0$, such that

$$\mathbb{T} \cup N_\epsilon(\boldsymbol{\theta}^*) = N_\epsilon(\boldsymbol{\theta}^*).$$

We then say that $\boldsymbol{\theta}^*$ is an **boundary point** of $\mathbb{T}$ if for all $\epsilon > 0$,

$$\mathbb{T} \cup N_\epsilon(\boldsymbol{\theta}^*) \neq N_\epsilon(\boldsymbol{\theta}^*).$$

We can extend the Weierstrass optimality theorem, as follows. If $\mathbb{T} \subset \mathbb{R}^d$ is compact and if $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is continuously differentiable, then there exists $\boldsymbol{\psi}, \boldsymbol{\upsilon} \in \mathbb{T}$, such that

$$f(\boldsymbol{\psi}) \leq f(\boldsymbol{\theta}) \leq f(\boldsymbol{\upsilon}),$$

for all $\theta \in \mathbb{T}$. Furthermore, if $\boldsymbol{\psi}$ or $\boldsymbol{\upsilon}$ are interior points, then they must be stationary points of f. If $\boldsymbol{\psi}$ or $\boldsymbol{\upsilon}$ are not stationary points, then they must be boundary points of f.

Convex sets

A set $\mathbb{T}$ is said to be **convex** if for all $\boldsymbol{\psi}, \boldsymbol{\upsilon} \in \mathbb{T}$, and for any $\lambda \in [0, 1]$, we have

$$\boldsymbol{\theta} = \lambda \boldsymbol{\psi} + (1 - \lambda) \boldsymbol{\upsilon} \in \mathbb{T}.$$

We say that $\boldsymbol{\theta}$ is a *convex combination* of the two points $\boldsymbol{\psi}$ and $\boldsymbol{\upsilon}$.

Some examples of convex sets in $\mathbb{R}^d$ include:

- The real space, $\mathbb{R}^d$, itself.
- Any *half space* $\{\boldsymbol{\theta} \in \mathbb{R}^d : \boldsymbol{a}^\top \boldsymbol{\theta} < b\}$, for $\boldsymbol{a} \in \mathbb{R}^d$ and $b \in \mathbb{R}$.
- Any *hyperplane* $\{\boldsymbol{\theta} \in \mathbb{R}^d : \boldsymbol{a}^\top \boldsymbol{\theta} = b\}$, for $\boldsymbol{a} \in \mathbb{R}^d$ and $b \in \mathbb{R}$.
- Any ball $\left\{\boldsymbol{\theta} \in \mathbb{R}^d : \|\boldsymbol{\theta} - \boldsymbol{\theta}^*\|_p < \epsilon\right\}$, for $\boldsymbol{\theta}^* \in \mathbb{R}^d$, $\epsilon > 0$, and $p \geq 1$.
- The intersection of any number of convex sets.

Convex functions

We say that the function $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is **convex**, over a convex domain $\mathbb{T}$, if for all $\psi, \upsilon \in \mathbb{T}$, and for any $\lambda \in [0, 1]$, we have

$$f(\lambda\psi + (1-\lambda)\upsilon) \leq \lambda f(\psi) + (1-\lambda) f(\upsilon).$$

The function f is said to be **strictly convex** if we change the symbol $\leq$ to the symbol $<$.

We then define a **concave** or **strictly concave** function by reversing the inequalities in the previous definitions.

It is not difficult to show that if f is a convex function, then $-f$ is a concave function, and *vice versa*.

The Hessian matrix and positive definiteness

Suppose that $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is now twice continuously differentiable over the convex domain $\mathbb{T}$.

Write the **Hessian** matrix of f at $\boldsymbol{\theta}^* \in \mathbb{T}$ as

$$\frac{\partial^2 f}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^\top}(\boldsymbol{\theta}^*) = \begin{bmatrix} \frac{\partial^2 f}{\partial \theta_1^2}(\boldsymbol{\theta}^*) & \frac{\partial^2 f}{\partial \theta_1 \partial \theta_2}(\boldsymbol{\theta}^*) & \cdots & \frac{\partial^2 f}{\partial \theta_1 \partial \theta_d}(\boldsymbol{\theta}^*) \\ \frac{\partial^2 f}{\partial \theta_1 \partial \theta_2}(\boldsymbol{\theta}^*) & \frac{\partial^2 f}{\partial \theta_2^2}(\boldsymbol{\theta}^*) & \cdots & \frac{\partial^2 f}{\partial \theta_2 \partial \theta_d}(\boldsymbol{\theta}^*) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial \theta_1 \partial \theta_d}(\boldsymbol{\theta}^*) & \frac{\partial^2 f}{\partial \theta_2 \partial \theta_d}(\boldsymbol{\theta}^*) & \cdots & \frac{\partial^2 f}{\partial \theta_d^2}(\boldsymbol{\theta}^*) \end{bmatrix}.$$

We say that a $d \times d$ matrix $\mathbf{A}$ is **positive definite** if for any $\boldsymbol{\theta} \in \mathbb{R}^d$, $\boldsymbol{\theta}^\top \mathbf{A} \boldsymbol{\theta} > 0$. A **positive semidefinite** matrix is defined by replacing the symbol $>$ by $\geq$. The definition for **negative definite** and **negative semidefinite** matrices are obtained by reversing the inequalities.

First and second order conditions

A continuously differentiable function $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is convex, over a convex domain $\mathbb{T}$, if for any $\boldsymbol{\psi}, \boldsymbol{\upsilon} \in \mathbb{T}$, such that $\boldsymbol{\psi} \neq \boldsymbol{\upsilon}$, we have

$$f(\boldsymbol{\psi}) \geq f(\boldsymbol{\upsilon}) + \left[\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\upsilon})\right]^{\top} (\boldsymbol{\psi} - \boldsymbol{\upsilon}).$$

We obtain strict convexity by replacing the symbol $\geq$ by $>$. First-order conditions for concavity and strict concavity are obtained by reversing the inequalities.

If f is twice continuously differentiable over the convex domain $\mathbb{T}$, then it is convex if its Hessian is positive semidefinite, for every $\boldsymbol{\theta}^* \in \mathbb{T}$. It is strictly convex if the Hessian is positive definite.

The definitions for concavity of a twice continuously differentiable function can be obtained by replacing the word *positive* by the word *negative*.

A third existence theorem

If $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is convex, over a convex domain $\mathbb{T}$, then a point $\boldsymbol{\theta}^* \in \mathbb{T}$ is a global minimizer if and only if

$$\left[\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*)\right]^\top (\boldsymbol{\psi} - \boldsymbol{\theta}^*) \geq 0,$$

for every $\boldsymbol{\psi} \in \mathbb{T}$.

Furthermore, if $\boldsymbol{\theta}^* \in \mathbb{T}$ is a local minimizer of f, then $\boldsymbol{\theta}^*$ is also a global minimizer of f. If f is strictly convex then it has at most one global minimizer.

Restatements of the results in terms of concave functions and maxima can be obtained by reversing the inequality.

The subdifferential

We now only assume that $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is convex. Denote the **subdifferential** of f at the point $\boldsymbol{\theta}^* \in \mathbb{T}$ by $\partial f(\boldsymbol{\theta}^*)$, where

$$\partial f(\boldsymbol{\theta}^*) = \left\{ \boldsymbol{\nu} \in \mathbb{R}^d : f(\boldsymbol{\theta}) \geq f(\boldsymbol{\theta}^*) + \boldsymbol{\nu}^\top (\boldsymbol{\theta} - \boldsymbol{\theta}^*), \text{ for all } \boldsymbol{\theta} \in \mathbb{T} \right\}.$$

When f is differentiable,

$$\partial f(\boldsymbol{\theta}^*) = \{(\partial f / \partial \boldsymbol{\theta})(\boldsymbol{\theta}^*)\}.$$

Using the notion of the subdifferential, we have the result that f has a global maximizer at $\boldsymbol{\theta}^*$ if and only if

$$\mathbf{0} \in \partial f(\boldsymbol{\theta}^*).$$

Notice, in the case of continuously differentiable f, that this condition reduces to

$$\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*) = \mathbf{0}.$$

Linear regression

Suppose that we observe responses $y_1, \ldots, y_n \in \mathbb{R}$ with companion covariates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$.

We wish to explain the relationship between any arbitrary $y \in \mathbb{R}$ and $\boldsymbol{x} \in \mathbb{R}^d$ via a hyperplane $\alpha + \boldsymbol{\beta}^\top \boldsymbol{x}$, such that

$$y \approx \alpha + \boldsymbol{\beta}^\top \boldsymbol{x},$$

in some sense.

The determination of the parameter $\boldsymbol{\theta}^\top = \left(\alpha, \boldsymbol{\beta}^\top\right) \in \mathbb{R}^{d+1}$ is known as the **linear regression** problem and can be solved in a number of ways.

We will firstly consider the method of *ridge-regularized least squares*, as proposed by Hoerl and Kennard (1970), where the parameter $\boldsymbol{\theta}$ is obtained by solving the problem

$$\min_{\boldsymbol{\theta}=(\alpha,\boldsymbol{\beta})\in\mathbb{R}^{d+1}} \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \alpha - \boldsymbol{\beta}^\top \boldsymbol{x}_i\right|_2^2 + \lambda \sum_{j=1}^{d} |\beta_j|_2^2 .$$

Matrix notation

Write $\overline{\boldsymbol{x}}_i^\top = (1, \boldsymbol{x}_i)$ and

$$\bar{\mathbf{I}} = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{bmatrix},$$

where $\mathbf{I}$ is the identity matrix of appropriate dimensionality, in order to obtain the expression

$$\begin{aligned} f(\boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} \left| y_i - \alpha + \boldsymbol{\beta}^\top \boldsymbol{x}_i \right|_2^2 + \lambda \sum_{j=1}^{d} |\beta_j|_2^2 \\ &= \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i \right)^2 + \lambda \boldsymbol{\theta}^\top \bar{\mathbf{I}} \boldsymbol{\theta}. \end{aligned}$$

If we further write $\mathbf{y}^\top = (y_1, \ldots, y_n)$ and let $\mathbf{X}$ be an $n \times d$ matrix with ith row $\overline{\boldsymbol{x}}_i^\top$, then we can further write

$$f(\boldsymbol{\theta}) = \frac{1}{n} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \boldsymbol{\theta}^\top \bar{\mathbf{I}} \boldsymbol{\theta}.$$

Solving the first order condition

We note that f is continuously differentiable in $\boldsymbol{\theta}$. Using the rules of matrix differentiation from the *Matrix Cookbook* of Petersen and Pedersen (2012), we can write the gradient at any point $\boldsymbol{\theta}$ as

$$\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}) = -\frac{2}{n}\mathbf{X}^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + 2\lambda\bar{\mathbf{I}}\boldsymbol{\theta},$$

which we can use to solve for a stationary point $\boldsymbol{\theta}^*$ that satisfies

$$\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*) = \mathbf{0}.$$

By solving the first order condition, we obtain the stationary point

$$\boldsymbol{\theta}^* = \left(\mathbf{X}^\top\mathbf{X} + n\lambda\bar{\mathbf{I}}\right)^{-1}\mathbf{X}^\top\mathbf{y}.$$

Rules of convexity

Assume that $\boldsymbol{\theta} \in \mathbb{T}$, where $\mathbb{T} \subseteq \mathbb{R}^d$ is convex. We can use the following rules for determining convexity (see Boyd and Vandenberghe (2004)):

- The (**affine**) function $f(\boldsymbol{\theta}) = \boldsymbol{a}^\top \boldsymbol{\theta} + b$ for $\boldsymbol{a} \in \mathbb{R}^d$ and $b \in \mathbb{R}$, is convex.
- The function $f(\theta) = \theta^2$ is convex.
- If $g(\cdot) : \mathbb{T} \to \mathbb{R}$ is affine and $h(\cdot) : \mathbb{R} \to \mathbb{R}$ is convex, then $f(\boldsymbol{\theta}) = h(g(\boldsymbol{\theta}))$ is convex.
- Positively weighted sums of convex functions is convex.

Checking convexity

Recall that

$$f(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \alpha - \boldsymbol{\beta}^\top \boldsymbol{x}_i\right|_2^2 + \lambda\sum_{j=1}^{d}|\beta_j|_2^2 .$$

By our third existence theorem, we can prove that $\boldsymbol{\theta}^*$ is a global minimizer if we can demonstrate that the objective function f is convex, in $\boldsymbol{\theta}$.

1. For each i, we know that $y_i - \alpha + \boldsymbol{\beta}^\top \boldsymbol{x}_i$ is affine, and thus convex.
2. Since $|\cdot|_2^2 = (\cdot)^2$, it is convex.
3. The affine compositions $\left|y_i - \alpha + \boldsymbol{\beta}^\top \boldsymbol{x}_i\right|_2^2$ and $|\beta_j|_2^2$ are convex, for each i and j.
4. Since, f is a positively weighted sum of convex functions, it is also convex.

We have therefore demonstrated that $\boldsymbol{\theta}^*$ is a global minimizer of f.

Robust ridge regression

Suppose now that we wish to solve the linear regression problem using a measurement of loss between each y_i and $\boldsymbol{x}_i$ that replaces the ℓ_2 loss by an ℓ_p loss, where $p \in [1, 2)$. In particular, we are interested in the case where $p = 1$ (*ridge regularized least-absolute deviation*).

Thus, we are interested in solving the problem

$$\min_{\boldsymbol{\theta}=(\alpha,\boldsymbol{\beta})\in\mathbb{R}^{d+1}} f(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \alpha - \boldsymbol{\beta}^\top \boldsymbol{x}_i\right|_p^p + \lambda\sum_{j=1}^{d}|\beta_j|_2^2 .$$

Unfortunately, f is no longer continuously differentiable, and thus we require an alternative approach to what we have used, previously.

The MM algorithm

Difficulties arising in optimization

Suppose that $f(\cdot) : \mathbb{T} \to \mathbb{R}$ is a difficult function to manipulate. We are interested in two particular types of difficulties:

1. The function f is not differentiable.
2. The function f is differentiable, but the solution to the first order condition

$$\frac{\partial f}{\partial \boldsymbol{\theta}}(\boldsymbol{\theta}^*) = \mathbf{0},$$

does not exist in closed form.

In such cases, we can operate on *surrogates* of f instead of operating on f, directly.

Majorization and minorization

Let $\psi, \theta \in \mathbb{T}$ and suppose that we wish to a approximate the behavior of f, evaluated at any $\psi \in \mathbb{T}$.

Introduce the function $\overline{f}(\cdot, \cdot) : \mathbb{T} \times \mathbb{T} \to \mathbb{R}$, and assume that $\overline{f}$ satisfies the properties:

1. For any $\theta \in \mathbb{T}$, $\overline{f}(\theta, \theta) = f(\theta)$.
2. For any $\psi \neq \theta$, $\overline{f}(\theta, \psi) \geq f(\theta)$.

We call such a function a **majorizer** of f, and for any fixed ψ, we say that $\overline{f}(\cdot, \psi) : \mathbb{T} \to \mathbb{R}$ **majorizes** f, at ψ.

The definition for a **minorizer** and the process of **minorization** can be obtained by reversing the inequality in the second condition.

A visualization of the majorization process

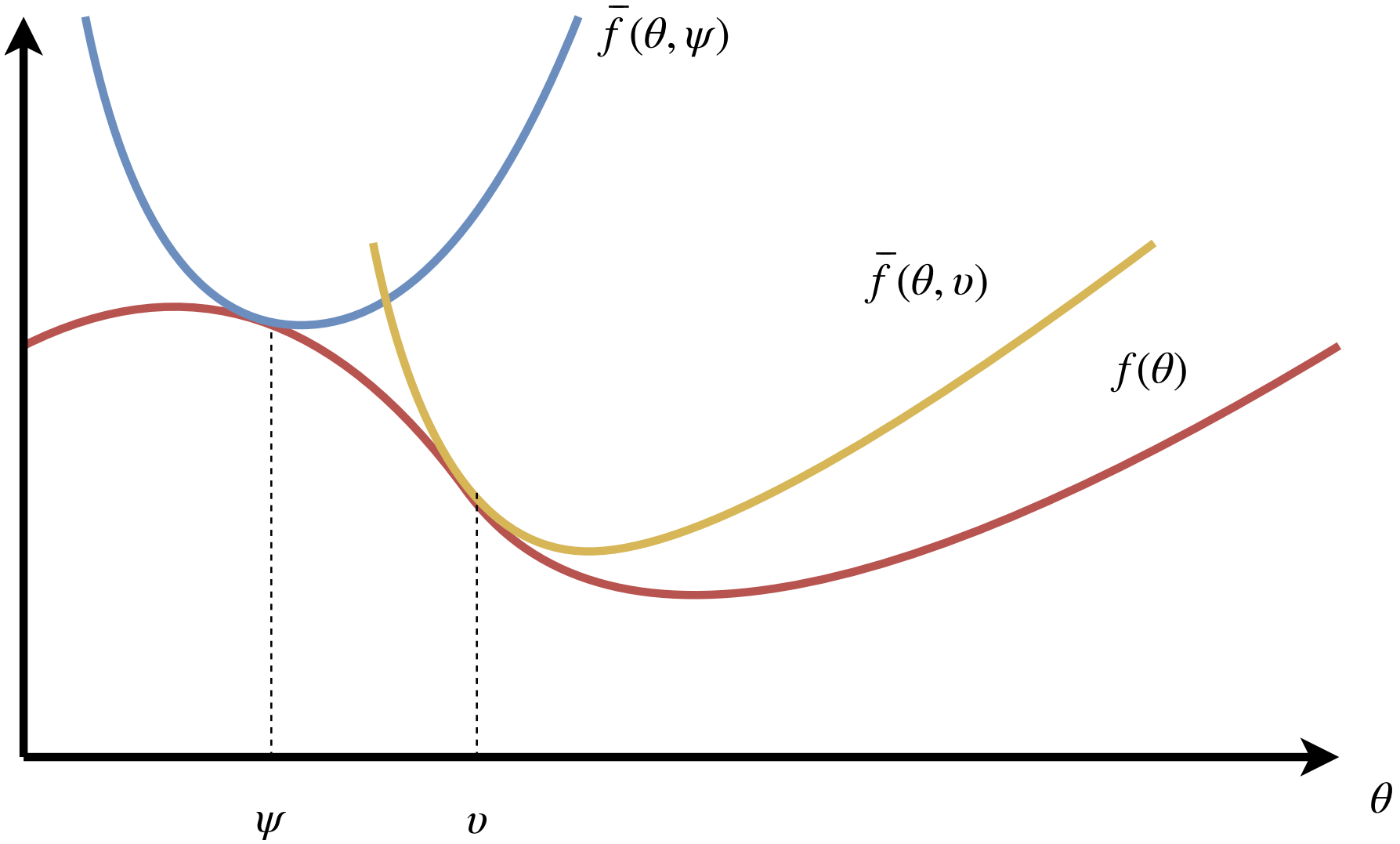


Figure 6: Example of majorizers of an arbitrary function.

The MM algorithm

Suppose that we wish to solve the minimization problem

$$\min_{\boldsymbol{\theta} \in \mathbb{T}} \; f\left(\boldsymbol{\theta}\right).$$

Let $\boldsymbol{\theta}^{(0)} \in \mathbb{T}$ be some **initialization** or *guess* of the solution to the problem. The **majorization-minimization** (**MM**) **algorithm** can be defined as follows. Let $\boldsymbol{\theta}^{(r)}$ be the be the rth iterate, obtained by the MM algorithm. We obtain this rth iterate by via the scheme

$$\boldsymbol{\theta}^{(r)} \in \left\{ \boldsymbol{\theta}^{*} \in \mathbb{T} : \overline{f}\left(\boldsymbol{\theta}^{*}, \boldsymbol{\theta}^{(r-1)}\right) = \min_{\boldsymbol{\theta} \in \mathbb{T}} \; \overline{f}\left(\boldsymbol{\theta}^{*}, \boldsymbol{\theta}^{(r-1)}\right) \right\}.$$

Alternatively, we can define the **minorization-maximization** (**MM**) **algorithm** for solving the problem

$$\max_{\boldsymbol{\theta} \in \mathbb{T}} \; f\left(\boldsymbol{\theta}\right),$$

via the scheme

$$\boldsymbol{\theta}^{(r)} \in \left\{ \boldsymbol{\theta}^{*} \in \mathbb{T} : \overline{f}\left(\boldsymbol{\theta}^{*}, \boldsymbol{\theta}^{(r-1)}\right) = \max_{\boldsymbol{\theta} \in \mathbb{T}} \; \overline{f}\left(\boldsymbol{\theta}^{*}, \boldsymbol{\theta}^{(r-1)}\right) \right\}.$$

Illustration of the MM algorithm

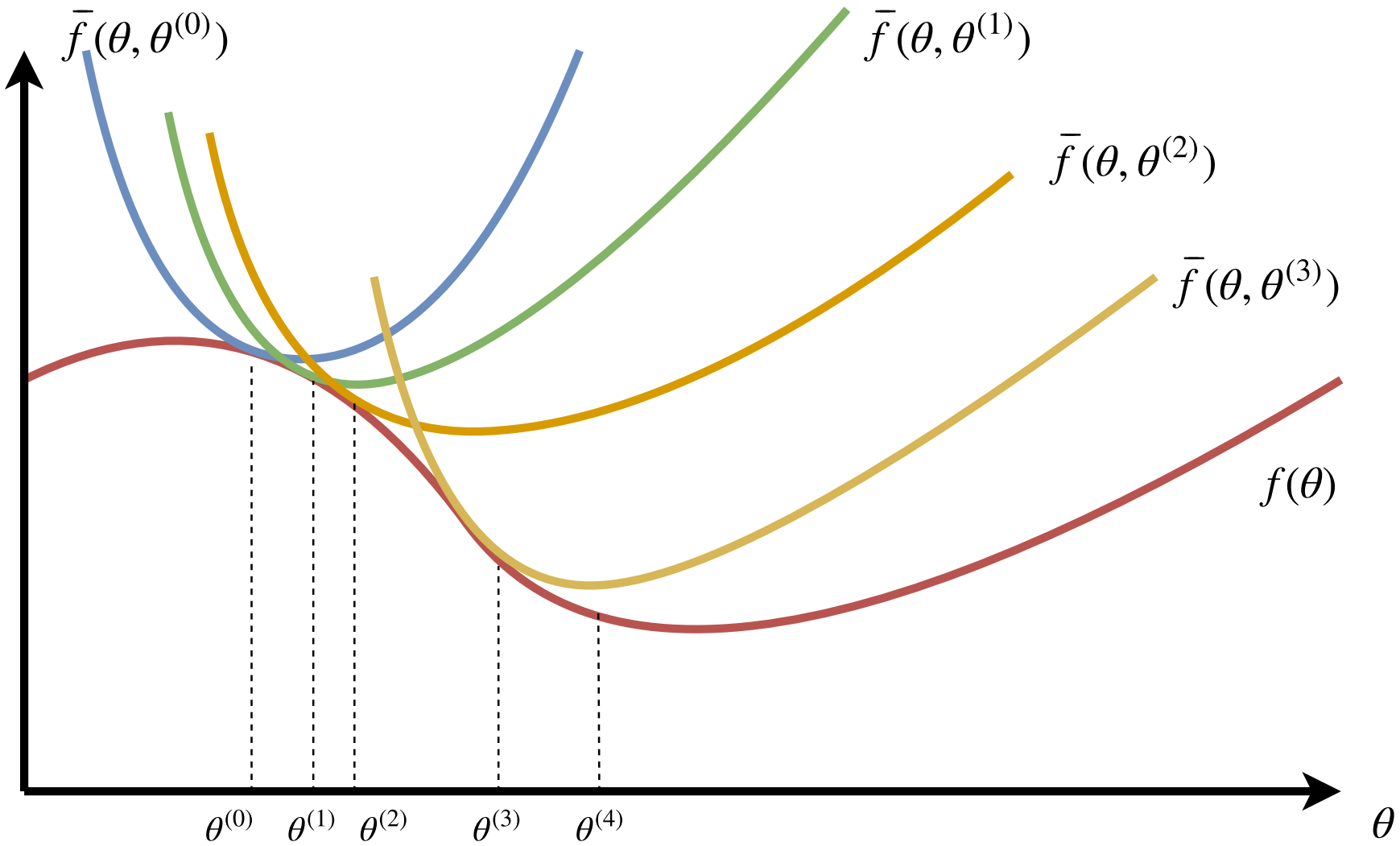


Figure 7: Four steps of an MM algorithm.

The descent property

Let $\boldsymbol{\theta}^{(r)}$ and $\boldsymbol{\theta}^{(r+1)}$ be two consecutive iterates of the MM algorithm, and recall that a majorizer $\overline{f}$ of f has the properties:

1. For any $\boldsymbol{\theta} \in \mathbb{T}$, $\overline{f}(\boldsymbol{\theta}, \boldsymbol{\theta}) = f(\boldsymbol{\theta})$.
2. For any $\boldsymbol{\psi} \neq \boldsymbol{\theta}$, $\overline{f}(\boldsymbol{\theta}, \boldsymbol{\psi}) \geq f(\boldsymbol{\theta})$.

By the first property, we have the equality

$$f\left(\boldsymbol{\theta}^{(r)}\right) = \overline{f}\left(\boldsymbol{\theta}^{(r)}, \boldsymbol{\theta}^{(r)}\right).$$

Since $\boldsymbol{\theta}^{(r+1)}$ minimizes $\overline{f}\left(\cdot, \boldsymbol{\theta}^{(r)}\right)$, we have

$$\overline{f}\left(\boldsymbol{\theta}^{(r)}, \boldsymbol{\theta}^{(r)}\right) \geq \overline{f}\left(\boldsymbol{\theta}^{(r+1)}, \boldsymbol{\theta}^{(r)}\right).$$

The second property then tells us that

$$\overline{f}\left(\boldsymbol{\theta}^{(r+1)}, \boldsymbol{\theta}^{(r)}\right) \geq f\left(\boldsymbol{\theta}^{(r+1)}\right),$$

and hence, for any $r \in \mathbb{N}$,

$$f\left(\boldsymbol{\theta}^{(r)}\right) \geq f\left(\boldsymbol{\theta}^{(r+1)}\right).$$

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