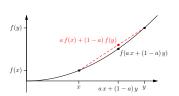
Advanced Machine Learning

Convexity



Convex sets, convex functions, Jensen's inequality

https://ecs-vlc.github.io/comp6208/

Convex Regions

• Convex regions are familiar



ullet For any two points x and y in a region ${\mathcal R}$ then for any $a \in [0,1]$ if



 $z = ax + (1 - a)y \in \mathcal{R}$

ullet then ${\mathcal R}$ is a convex region

https://ecs-vlc.github.io/comp6208/

Positive Semi-Definite Matrices

ullet Recall that a matrix M is positive semi-definite if for any vector v

$$\boldsymbol{v}^\mathsf{T} \mathbf{M} \boldsymbol{v} \ge 0$$

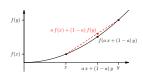
(i.e. any quadratic form of the matrix is non-negative)

- (We showed this also implies that all the eigenvalues are non-negative)
- ullet We denote the fact that $oldsymbol{M}$ is positive semi-definite by $oldsymbol{M}\succeq 0$, and $\mathbf{M}\succ 0$ if it is positive definite
- The set of positive semi-definite (PSD) matrices (or kernels) form a convex set

COMP6208 Advanced Machine Learning

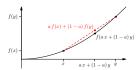
Outline

- 1 Convex sets
- 2. Convex functions
- 3. Jensen's inequality



1 Convex sets

- 2. Convex functions
- 3. Jensen's inequality



Convex Sets

Outline

ullet For any set, \mathcal{S} , where addition and scalar multiplication is defined (e.g. a vector space) then:

If for any two elements $x,y \in \mathcal{S}$ and any $a \in [0,1]$

$$z = ax + (1 - a)y \in S$$

then ${\mathcal S}$ is said to be a convex set

Proof

ullet Consider any two arbitrarily chosen PSD matrices M_1 and M_2 and any $a \in [0,1]$ then let

$$\mathbf{M}_3 = a\mathbf{M}_1 + (1-a)\mathbf{M}_2$$

ullet Then for any vector $oldsymbol{v}$

$$egin{aligned} oldsymbol{v}^\mathsf{T} \mathbf{M}_3 oldsymbol{v} &= oldsymbol{v}^\mathsf{T} (a \mathbf{M}_1 + (1-a) \mathbf{M}_2) oldsymbol{v}^\mathsf{T} \\ &= a oldsymbol{v}^\mathsf{T} \mathbf{M}_1 oldsymbol{v} + (1-a) oldsymbol{v}^\mathsf{T} \mathbf{M}_2 oldsymbol{v}^\mathsf{T} \\ &= a m_1 + (1-a) m_2 \end{aligned}$$

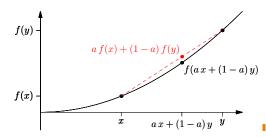
where $m_1 = oldsymbol{v}^\mathsf{T} \mathbf{M}_1 oldsymbol{v}$ and $m_2 = oldsymbol{v}^\mathsf{T} \mathbf{M}_2 oldsymbol{v}$

• But $m_1, m_2 \ge 0$ since $\mathbf{M}_1, \mathbf{M}_2 \succeq 0$. Thus $am_1 + (1-a)m_2 \ge 0$ and so $M_3 \succeq 0$

Convex Functions

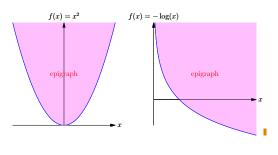
• Any function f(x) is said to be a **convex function** if for any two points x and y and any $a \in [0,1]$

$$f(ax + (1-a)y) \le af(x) + (1-a)f(y)$$



Epigraph

- The epigraph of a function is the area that lies above the function
- The epigraph of a convex function is a convex region

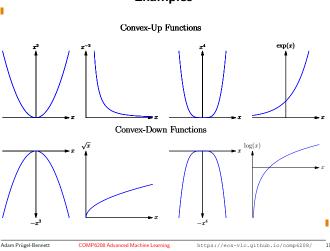


Adam Prügel-Bennet

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Examples



Strictly Convex Function

 Functions that satisfy the strict inequality (for 0 < a < 1 and $x \neq y)$

$$f(ax + (1 - a)y) < af(x) + (1 - a)f(y)$$

are said to be strictly convex functions

- A strictly convex-down function satisfies the reverse strict inequality
- Strictly convex-(up or down) functions don't contain any linear regions

Adam Prügel-Bennett

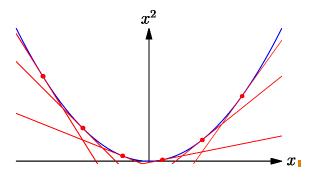
COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Properties of Convex Functions

• Convex functions lie on or above any tangent line

$$f(x) \ge f(x^*) + (x - x^*)f'(x^*)$$



Convex-Down or Concave Functions

• Any function, f(x), that satisfies the inverse inequality

$$f(ax + (1-a)y) \ge af(x) + (1-a)f(y)$$

for any points x and y and any $a \in [0,1]$ is said to be a **convex-down** or **concave** function

- Everything true for a convex(-up) function carries over to a convex-down function with a small modification
- If f(x) is a convex-up function then g(x) = -f(x) is a convex-down function
- The area that lies below a convex-down function is a convex region

Adam Prügel-Bennett

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Linear Functions

• Linear functions are given by

$$f(x) = mx + c\mathbf{I}$$

• They satisfy the equality

$$f(ax+(1-a)y)=af(x)+(1-a)f(y) \mathbb{I}$$

• As such they are both convex(-up) and convex-down function



Adam Prügel-Benner

COMP6208 Advanced Machine Learni

https://ecs-vlc.github.io/comp6208/

Convexity in High Dimensions

• If $f:\mathbb{R}^n \to \mathbb{R}$ (i.e. f(x) maps high dimensional point $x \in \mathbb{R}^n$ to a real value) satisfies

$$f(a\boldsymbol{x} + (1-a)\boldsymbol{y}) \le af(\boldsymbol{x}) + (1-a)f(\boldsymbol{y})$$

for any $x,y\in\mathbb{R}^n$ and any $a\in[0,1]$ then f(x) is a convex function!

- $\| {m x} \|_2^2 = \sum_i x_i^2$ is a (strictly) convex function
- ullet $\|x\|_1 = \sum\limits_i |x_i|$ is a convex function

Adam Prügel-Bennett

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Second Derivatives

ullet As f(x) lies on or above its tangent line then for any $\epsilon>0$

$$f'(x+\epsilon) \ge f'(x)$$

therefore $f''(x) = \lim_{\epsilon \to 0} (f'(x+\epsilon) - f'(x))/\epsilon \ge 0$ at all points x

• In high dimensions a convex function lies above its tangent plane

$$f(oldsymbol{x}) \geq f(oldsymbol{x}^*) + (oldsymbol{x} - oldsymbol{x}^*)^\mathsf{T} oldsymbol{
abla} f(oldsymbol{x})$$

 \bullet The matrix of second derivatives (the Hessian) must be positive semi-definite at all points \boldsymbol{x}

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_2} & \dots \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2^2} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \succeq 0$$

Adam Prügel-Bennett COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Adam Prügel-Bennett

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Proving Convexity

- $f(x) = x^2$ is strictly convex as f''(x) = 2 > 0
- $f(x) = e^{cx}$ is strictly convex as $f''(x) = c^2 e^{cx} > 0$
- $f(x) = \log(x)$ is strictly convex-down as $f''(x) = -\frac{1}{x^2} < 0$
- $f(x,y) = \frac{x^2}{y}$ is convex for y > 0 as

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 f(x,y)}{\partial x^2} & \frac{\partial^2 f(x,y)}{\partial x \partial y} \\ \frac{\partial^2 f(x,y)}{\partial y \partial x} & \frac{\partial^2 f(x,y)}{\partial y^2} \end{pmatrix} = \begin{pmatrix} \frac{2}{y} & -\frac{2x}{y^2} \\ -\frac{2x}{y^2} & \frac{2x^2}{y^3} \end{pmatrix} = \frac{2}{y^3} \begin{pmatrix} y^2 & -xy \\ -xy & x^2 \end{pmatrix} \mathbf{I}$$

- Now $T=\mathrm{tr}\mathbf{H}=\frac{2}{v^3}(x^2+y^2)$, $D=\det(\mathbf{H})=0$
- $\bullet \ \lambda_{1,2} = T/2 \pm \sqrt{T^2/4 D} = \{0,T\} = \{0,\frac{2(x^2 + y^2)}{y^3}\} \geq 0 \Rightarrow \mathbf{H} \succeq 0 \mathbf{I}$

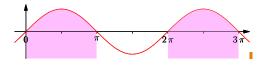
Adam Prügel-Bennet

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Convex Functions Defined on Convex Sets

- All the properties we have discussed hold for functions defined on a convex set!
- $\sin(x)$ is not generally neither convex up or down
- $\sin(x)$ for $x \in [0,\pi]$ is convex-down! (its second derivative $-\sin(x)$ is less than or equal to 0 in this range)!



• For a convex function defined on a non-convex set, \mathcal{S} , there exists points $x,y\in\mathcal{S}$ such that for some $a\in[0,1]$ there will be points $z=ax+(1-a)y\not\in\mathcal{S}$ (the function isn't defined on such points)

Adam Prügel-Bennet

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Unique Minimum

- Strictly convex function have a unique minimum
- The existence of a local minimum would break convexity
 - ★ The line connecting a local minimum to a global minimum would be strictly decreasing
 - ★ Thus there are points next to the local minimum with lower values



- ★ This is a contradiction
- This remains true if we consider convex functions that are constrained to live in a convex set!

Adam Prügel-Benne

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Linear Regression

• For linear regression the loss function

$$L(\boldsymbol{w}) = \|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 = \boldsymbol{w}^\mathsf{T}\mathbf{X}^\mathsf{T}\mathbf{X}\boldsymbol{w} - 2\boldsymbol{w}^\mathsf{T}\mathbf{X}^\mathsf{T}\boldsymbol{y} + \boldsymbol{y}^\mathsf{T}\boldsymbol{y}$$

is convey

- Since the Hessian $\mathbf{H} = 2\mathbf{X}^{\mathsf{T}}\mathbf{X} \succeq 0$ (positive semi-definite) (For any vector \mathbf{v} then $\mathbf{v}^{\mathsf{T}}\mathbf{H}\mathbf{v} = 2\mathbf{v}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\mathbf{v} = 2\|\mathbf{X}\mathbf{v}\|^2 \geq 0$)
- If $H \succ 0$ there will be a unique minimal while if H has some zero eigenvalues there will be a family of solutions

Sums of Convex Functions

ullet For any set of convex functions $f_1(x)$, $f_2(x)$, ... and any set of non-negative scalars $a_1,\ a_2,\ \dots$ then

$$g(x) = \sum_{i} a_i f_i(x)$$

is convex

Proof

$$g''(x) = \sum_{i} a_i f_i''(x)$$

but $f_i''(x) \ge 0$ so g''(x) is a sum on non-negative terms

 This generalises to higher dimensions as the sum of PSD matrices times positive factors is a PSD matix

Adam Prügel-Bennett

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Constraints

Often we impose constraints on the set of points, e.g.

$$x_i > 0$$
 $a^\mathsf{T} x = b$ $x^\mathsf{T} M x \le 1$

- Linear constraints (e.g. $x_i>0$ or ${\pmb a}^{\sf T}{\pmb x}=b$ or ${\pmb a}^{\sf T}{\pmb x}\le b$) always define a convex region
- Multiple linear constraints always define a convex region
- Non-linear constraints may or may not define a convex region $(\{ \boldsymbol{x} \in \mathbb{R}^n | \boldsymbol{x}^\mathsf{T} \mathbf{M} \boldsymbol{x} \leq 1, \mathbf{M} \succeq 0 \} \text{ does while } \\ \{ \boldsymbol{x} \in \mathbb{R}^n | \boldsymbol{x}^\mathsf{T} \mathbf{M} \boldsymbol{x} \geq 1, \mathbf{M} \succeq 0 \} \text{ doesn't}) \textbf{I}$

Adam Prügel-Bennett

COMP6208 Advanced Machine Learni

https://ecs-vlc.github.io/comp6208/

Convex Set of Minima

- If f(x) is **convex** but not **strictly convex** then there might exist a convex set $\mathcal{M} \subset \mathcal{X}$ of minima such that for all $x,y \in \mathcal{M}$ and any $z \in \mathcal{X}$ we have $f(x) = f(y) \leq f(z) \mathbb{I}$
- This set of minima is convex, that is, if $x,y\in\mathcal{M}$ then for any $a\in[0,1]$ the point $z=ax+(1-a)y\in\mathcal{M}$
- The sum of a convex function, f(x), and a strictly convex function g(x) will always be strictly convex since

$$f''(x) + g''(x) > 0$$

as $f''(x) \ge 0$ and g''(x) > 0

Adam Prügel-Bennett

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Regularised Linear Regression

• In ridge regression we minimise a loss

$$L(\boldsymbol{w}) = \|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 + \eta \|\boldsymbol{w}\|^2 = \boldsymbol{w}^{\mathsf{T}} (\mathbf{X}^{\mathsf{T}} \mathbf{X} + \eta \mathbf{I}) \boldsymbol{w} - 2 \boldsymbol{w}^{\mathsf{T}} \mathbf{X}^{\mathsf{T}} \boldsymbol{y} + \boldsymbol{y}^{\mathsf{T}} \boldsymbol{y}^{\mathsf{T}}$$

- ullet Because $\|w\|^2$ is strictly convex the loss function is strictly convex and so will have a unique solution
- Using an L_1 regulariser (Lasso)

$$L(w) = \|Xw - y\|^2 + \eta \|w\|_1$$

again $\| \boldsymbol{w} \|_1$ is convex and so $L(\boldsymbol{w})$ will be convex

 Using an L₁ and an L₂ regulariser (elastic net) also gives a unique solution

Adam Prügel-Bennett

COMP6208 Advanced Machine Learning

https://ecs-vlc.github.io/comp6208/

Adam Prügel-Bennett

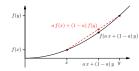
COMP6208 Advanced Machine Learn

https://ecs-vlc.github.io/comp6208/

Outline

1. Convex sets

- 2. Convex functions
- 3. Jensen's inequality



Adam Prügel-Bennet

COMPONE ALL IN III I

https://ecs-vlc.github.io/comp6208/

Proof

• We said before that a convex function must lie on or above its tangent plane at any point \boldsymbol{x}^*

$$f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*) + (\boldsymbol{x} - \boldsymbol{x}^*)^\mathsf{T} \nabla f(\boldsymbol{x}^*)$$

ullet Taking $oldsymbol{x}^* = \mathbb{E}[oldsymbol{X}]$

$$f(\boldsymbol{X}) \geq f(\mathbb{E}[\boldsymbol{X}]) + (\boldsymbol{X} - \mathbb{E}[\boldsymbol{X}])^\mathsf{T} \boldsymbol{\nabla} f(\mathbb{E}[\boldsymbol{X}]) \mathbf{I}$$

• Taking expectations of both sides

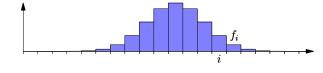
$$\begin{split} \mathbb{E}[f(X)] &\geq f(\mathbb{E}[X]) + (\mathbb{E}[X] - \mathbb{E}[X])^\mathsf{T} \nabla f(\mathbb{E}[X]) \mathbf{I} \\ &= f(\mathbb{E}[X]) \end{split}$$

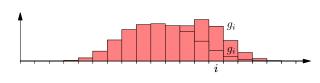
Adam Prügel-Bennett

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Kullback-Leibler Divergence





$$\mathrm{KL}(\boldsymbol{f}\|\boldsymbol{g}) = -\sum_{i=1}^{n} f_i \, \log \left(\frac{g_i}{f_i}\right) = 0.235$$

Adam Prügel-Bennet

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Lessons

- Although we haven't talked much about machine learning, convexity is heavily used in many machine learning applications
- A lot of ML algorithms involve convex functions e.g. SVMs
- As such they will have a unique minimum (or a convex set of minima)
- Convexity is an elegant idea which is relatively easy to prove theorems about
- One of the most useful tools is Jensen's inequality

Jensen's Inequality

- In proving many properties of learning machines inequalities are really useful
- One of the most useful inequalities involve expectations of convex functions, this is known as Jensen's Inequality
- ullet If $f(oldsymbol{x})$ is a convex(-up) function then

$$\mathbb{E}[f(\boldsymbol{X})] \geq f(\mathbb{E}[\boldsymbol{X}]) \mathbf{I}$$

• If f(x) is a convex(-down) function then

$$\mathbb{E}[f(\boldsymbol{X})] \leq f(\mathbb{E}[\boldsymbol{X}]) \mathbf{I}$$

Adam Prügel-Benne

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Simple Proofs with Jensen's Inequality

ullet Since $f(x)=x^2$ is convex by Jensen's inequality

$$\mathbb{E}\big[X^2\big] \geq (\mathbb{E}[X])^2 \mathbb{I} \quad \text{or} \quad \mathbb{E}\big[X^2\big] - \mathbb{E}[X]^2 \geq 0$$

(i.e. variance are non-negative)

• The KL-divergence $\mathrm{KL}(f\|g)$ between two categorical probability distributions (f_1,f_2,\ldots) and (g_1,g_2,\ldots) is define as

$$KL(f||g) = -\sum_{i} f_i \log\left(\frac{g_i}{f_i}\right)$$

(note $f_i,g_i\geq 0$ and $\sum\limits_i f_i=\sum\limits_i g_i=1$)

Adam Prügel-Bennett

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/

Proof of Gibbs' Inequality

• To show that $\mathrm{KL}(f\|g) \geq 0$ (Gibbs' inequality) we note that since the logarithm is a convex-down function

$$\begin{split} \mathrm{KL}(f \| g) &= -\sum_i f_i \log \left(\frac{g_i}{f_i} \right) \mathbb{I} = \mathbb{E}_f \bigg[-\log \left(\frac{g_i}{f_i} \right) \bigg] \mathbb{I} \\ &\geq -\log \bigg(\mathbb{E}_f \left[\frac{g_i}{f_i} \right] \bigg) \mathbb{I} \\ &= -\log \bigg(\sum_i f_i \frac{g_i}{f_i} \bigg) \mathbb{I} = -\log \bigg(\sum_i g_i \bigg) \mathbb{I} = -\log (1) \mathbb{I} = 0 \mathbb{I} \end{split}$$

• We will meet KL-divergences later on

Adam Prügel-Bennet

COMP6208 Advanced Machine Learnin

https://ecs-vlc.github.io/comp6208/