Ch2. Mathematical Toolbox

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Outline

Scalar product

- For $u, v \in \mathbb{R}^d$ the scalar product is defined as

$$\langle u, v \rangle = \sum_{i=1}^{d} u_i \, v_i = u^\top \, v$$

- For $u, v \in \mathbb{R}^d$ and matrix $A \in \mathbb{R}^{d \times d}$

$$\langle u, Av \rangle = \sum_{1 \leq i,j \leq d} A_{i,j} u_i v_j = u^\top \, A \, v$$

- For $u \in \mathbb{R}^p$, $v \in \mathbb{R}^q$, and matrix $A \in \mathbb{R}^{p \times q}$

$$\langle u, Av \rangle = \left\langle A^\top u, v \right\rangle$$

Inverse

- For two matrices A, B we have

$$(A\,B)^\top = B^\top\,A^\top \qquad \text{and} \qquad (A\,B)^{-1} = B^{-1}\,A^{-1}$$

- **[Exercise]** transpose and inverse interact as follows

$$\left(A^\top\right)^{-1} = \left(A^{-1}\right)^\top$$

Determinant

- The determinant satisfies the identity

$$\det(A\,B) = \det(A)\,\det(B) \qquad \text{and} \qquad \det(A^{-1}) = (\det(A))^{-1}\,.$$

- The determinant of a triangular matrix is the product of the elements on the diagonal

$$\det\begin{pmatrix} 2 & & \\ 6 & 1 & \\ -8 & 5 & 3 \end{pmatrix} = 2 \times 1 \times 3 = 6$$

Orthogonal matrices

- A matrix $O \in \mathbb{R}^{d\times d}$ is called orthogonal if $O\,O^\top = I$.
- Equivalently, a matrix $O \in \mathbb{R}^{d\times d}$ is orthogonal if $O^{-1} = O^\top$.
- Equivalently, a matrix $O \in \mathbb{R}^{d\times d}$ is orthogonal if it rows (or column) have norm 1 and are perpendicular.
- If O is orthogonal, for any vector v we have

$$\|O\,v\| = \|v\|.$$

- **[Exercise]** prove that the following is orthogonal

$$O = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

Symmetric matrices

- A matrix $S \in \mathbb{R}^{d\times d}$ is called symmetric if $M_{i,j} = M_{j,i}$ for all $1 \le i,j \le d$.
- A symmetric matrix M is diagonalizable in an orthogonal matrix,

$$M = O\,D\,O^\top$$

for an orthogonal matrix O and a diagonal matrix $D = \mathrm{Diag}(\lambda_1,\ldots,\lambda_d)$. The $\{\lambda_i\}_{i=1}^d$ are the eigenvalues of M.

Positive Symmetric matrices

- A symmetric matrix $S \in \mathbb{R}^{d\times d}$ is positive semi-definite if for any vector $v \in \mathbb{R}^d$ we have
$$\langle x, Sx\rangle \geq 0.$$
Caution: elements of S do not need to be non-negative.
- **[Exercise]** a covariance matrix is positive semi-definite.
- **[Exercise]** the sum of two positive definite matrices is positive definite
- A symmetric matrix $S \in \mathbb{R}^{d\times d}$ is positive definite if for any vector $v \neq 0$ we have
$$\langle x, Sx\rangle > 0.$$
- Symmetric matrix S is positive definite if $\lambda_i > 0$ for all i.

Example

- **[Exercise]** is the matrix

$$M = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

positive definite? Is it positive semi-definite?

- A symmetric positive definite matrix S can always be decomposed as
$$S = L\,L^\top$$
where L is a lower triangular matrix. This is the Cholesky decomposition of S.

- For example,
$$S = \begin{pmatrix} 4 & 12 & -16 \\ 12 & 37 & -43 \\ -16 & -43 & 98 \end{pmatrix} = \begin{pmatrix} 2 & & \\ 6 & 1 & \\ -8 & 5 & 3 \end{pmatrix} \begin{pmatrix} 2 & 6 & -8 \\ & 1 & 5 \\ & & 3 \end{pmatrix}$$

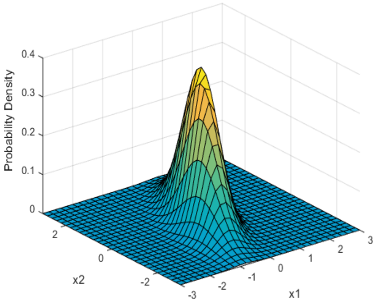
- **[Exercise]** compute the determinant of S.

Outline

Multivariate Gaussian Density

- A Gaussian distribution in $\mathbb{R}^d$ with mean $\mu \in \mathbb{R}^d$ and covariance $\Gamma \in \mathbb{R}^{d\times d}$ has density, if Γ is invertible, given by

$$\frac{1}{(2\,\pi)^{d/2}\ \det(\Gamma)^{1/2}} \times \exp\left\{-\frac{1}{2}\left\langle [x-\mu], \Gamma^{-1}\,[x-\mu]\right\rangle\right\}$$



Multivariate Gaussian Density

- If ξ is a Gaussian random variable in $\mathbb{R}^d$ with mean $\mu \in \mathbb{R}^d$ and covariance $\Gamma \in \mathbb{R}^{d\times d}$ then for a matrix $A \in \mathbb{R}^{n\times d}$ and vector $b \in \mathbb{R}^n$ the random variable $Y = A\,\xi + b$ has means

$$\mathrm{Mean}(Y) = A\,\mu + b$$

and covariance

$$\mathsf{Cov}(Y) = A\,\Gamma\,A^\top$$

- Let $\Gamma \in \mathbb{R}^{d\times d}$ be a covariance matrix and $\mu \in \mathbb{R}^d$. Consider the Cholesky decomposition

$$\Gamma = L\,L^\top.$$

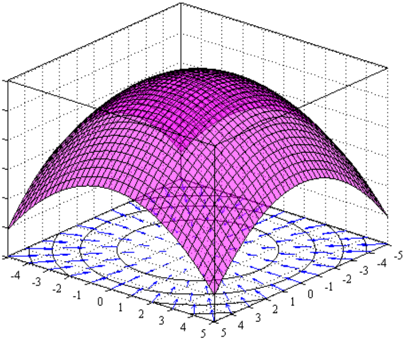
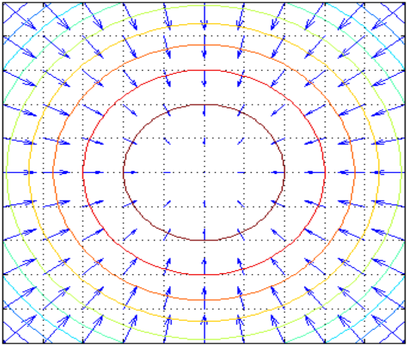
[**Exercise**] the random variable $\xi = L\,\zeta + \mu$, with $\zeta = \mathbf{N}\,(0, I_d)$ is a Gaussian random variable with mean μ and covariance Γ.

Outline

- Consider a function $f : \mathbb{R}^d \to \mathbb{R}$. The gradient is defined as

$$\nabla f(x) = (\partial_{x_1} f(x), \ldots, \partial_{x_d} f(x))$$

- Intuitively: $f(x+\varepsilon) \approx f(x) + \langle \nabla f(x), \varepsilon \rangle$
- Example: $f(x) = -\frac{1}{2}\ (x_1^2 + \ldots + x_d^2)$.

Gradient: important examples

- Let $v \in \mathbb{R}^d$ and $f(x) = \langle v, x \rangle$,

$$\nabla f(x) = \dots$$

- Let $M \in \mathbb{R}^{d \times d}$ and $g(x) = \frac{1}{2} \langle x, Mx \rangle$,

$$\nabla g(x) = \dots$$

Hessian matrix

- Let $f : \mathbb{R}^d \to \mathbb{R}$ be a function
- The Hessian of f at x is the matrix $\mathrm{Hess}(x) \in \mathbb{R}^{d\times d}$ defined as

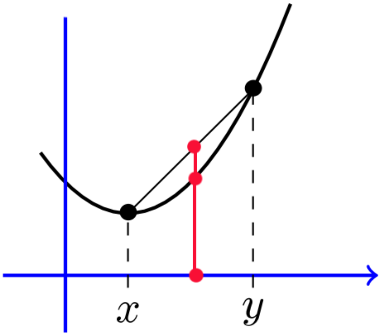
$$\mathrm{Hess}(x)_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}(x)$$

- Intuitively: $f(x+\varepsilon) \approx f(x) + \langle \nabla f(x), \varepsilon \rangle + \frac{1}{2}\, \langle \varepsilon, \mathrm{Hess}(x)\, \varepsilon \rangle$
- [**Exercise**] what is the Hessian of $f(x) = \frac{1}{2}\, \langle x, Mx \rangle$

Outline

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if for any $x, y \in \mathbb{R}^d$ and $0 < \lambda < 1$ we have

$$f\left(\lambda\, x + (1-\lambda)\, y\right) \leq \lambda\, f\left(x\right) + (1-\lambda)\, f\left(y\right).$$



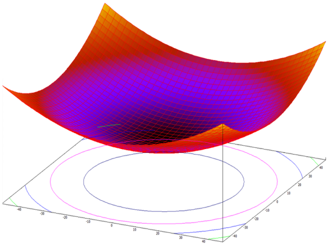
Strict Convexity

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is strictly convex if for any $x \neq y \in \mathbb{R}^d$ and $0 < \lambda < 1$ we have

$$f\left(\lambda\, x + (1-\lambda)\, y\right) < \lambda f\left(x\right) + (1-\lambda) f\left(y\right).$$

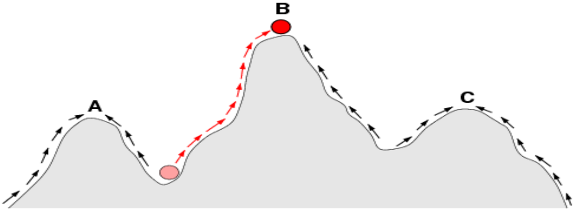
Convex function: second derivative criterion

- Consider a function $f : \mathbb{R}^d \to \mathbb{R}$.
- If the Hessian matrix $\mathrm{Hess}(x)$ is positive semi-definite for every $x \in \mathbb{R}^d$ then the function is convex.
- If the Hessian matrix $\mathrm{Hess}(x)$ is positive definite for every $x \in \mathbb{R}^d$ then the function is strictly convex.

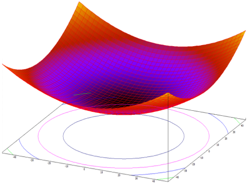


- **[Exercise]** the sum of two convex functions is convex

Optimization and Convexity



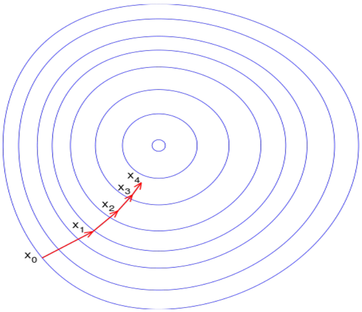
- If a strictly convex function has a local minimum, this minimum is the unique global minimum.

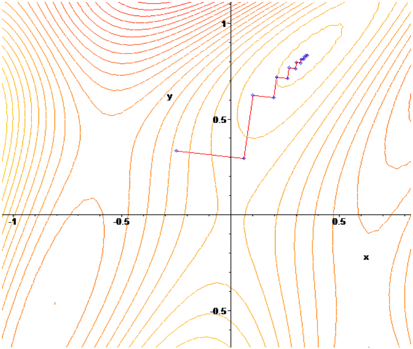


Gradient descent

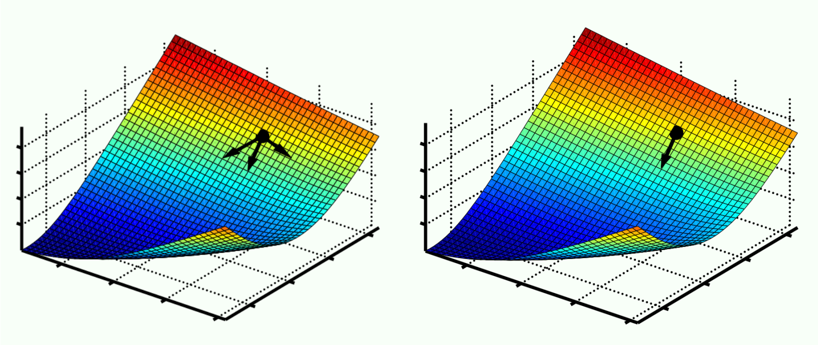
- Consider $f : \mathbb{R}^d \to \mathbb{R}$ a function to minimize.
- For a learning rate $\eta > 0$ (or step-size) the gradient descent algorithm is as follows,

$$x_{n+1} = x_n - \eta \nabla f(x_n)$$

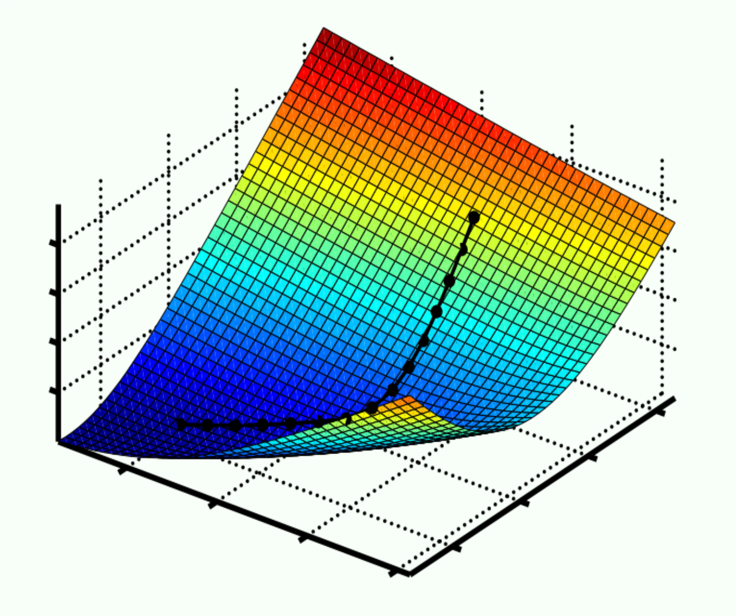




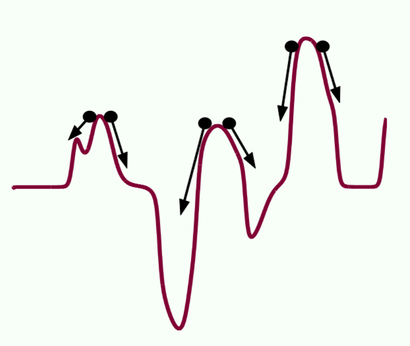
Gradient descent



Gradient descent



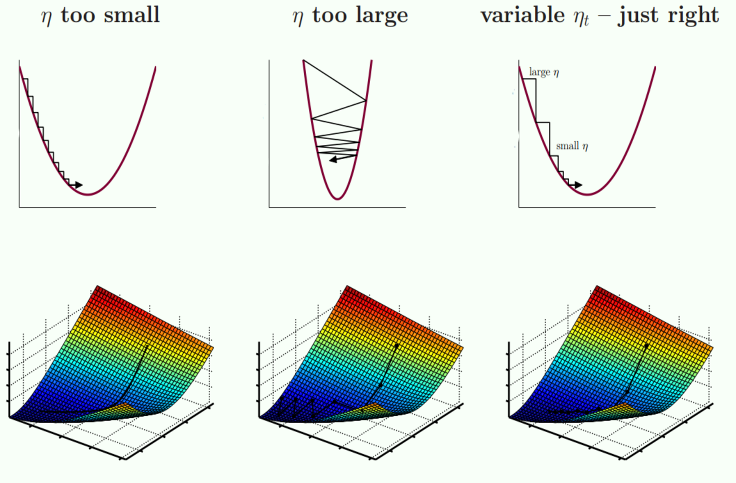
Gradient descent can get stuck!



This cannot happen when optimizing a convex function!

On the Learning Rate

- Gradient descent reads $x_{n+1} = x_n - \eta \nabla f(x_n)$.
- [**Exercise**] Gradient descent for $f(x) = \frac{1}{2}x^2$: influence of η?



Gradient descent

- We would like to solve the equation $A\,x = b$ for a positive definite matrix $A \in \mathbb{R}^d$.
- Consider the

$$f(x) = \frac{1}{2}\,\left\langle A\,x - b, A^{-1}(Ax - b)\right\rangle$$

- **[Exercise]** prove that the function f is strictly convex.
- **[Exercise]** prove that the solution $x^\star$ of $A\,x = b$ is the unique global minimum of f.
- **[Exercise]** write the gradient descent algorithm for minimizing the function f.

Outline

Performance and Loss function

- Performance of a parameter θ can be quantified by

$$F(\theta) = \frac{1}{N} \sum_{i=1}^{N} \textsf{\textbf{Loss}}(\theta, x_i, y_i) + \Omega(\theta)$$

where

  - **Loss**$(\,\cdot\,)$ quantifies the fit to the data
  - $\{x_i, y_i\}_{i=1}^{N}$ are training examples
  - $\Omega(\theta)$ is a regularisation term

- One would to minimise the function F,

$$\widehat{\theta} = \mathbf{argmax}\ F(\theta)$$

Regularized Linear Regression

- In linear regression, the least square estimate $\widehat{\beta}$ minimises the function
$$F(\beta) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \langle x_i, \beta\rangle\right)^2 .$$
Note that there is no regularisation term.
- For ridge regression, the estimate $\widehat{\beta}_{\text{ridge}}$ minimises
$$F_{\text{ridge}}(\beta) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \langle x_i, \beta\rangle\right)^2 + \lambda \sum_{i=1}^{d} \beta_i^2$$
[**Exercise**] find $\nabla F_{\text{ridge}}(\beta)$.
- For LASSO regression, the estimate $\widehat{\beta}_{\text{lasso}}$ minimises
$$F_{\text{ridge}}(\beta) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \langle x_i, \beta\rangle\right)^2 + \lambda \sum_{i=1}^{d} |\beta_i|$$

Regularized Logistic Regression

- Training examples: $\{x_i, y_i\}_{i=1}^N$ with $x_i \in \mathbb{R}^d$
- $y_i \in \{+1, -1\}$
- Regularized logistic regression: $\widehat{\beta} \in \mathbb{R}^d$ minimises

$$F(\beta) = \frac{1}{N} \sum_{i=1}^{N} \log\left(1 + e^{-y_i \langle x_i, \beta \rangle}\right) \; + \; \lambda \sum_{i=1}^{d} \beta_i^2$$

- **[Exercise]** write down the gradient descent update for fitting a regularized logistic regression.
- **[Exercise]** the function $\beta \mapsto F(\beta)$ is convex.

Stochastic Gradient Descent

- If $N \gg 1$, computing the gradient of F can be expensive,

$$\nabla F(\beta) = \frac{1}{N} \sum_{i=1}^{N} \nabla \textbf{Loss}(\beta, x_i, y_i) \; + \; \nabla \Omega(\beta)$$

- stochastic gradient: replace $\frac{1}{N} \sum_{i=1}^{N}$ by $\frac{1}{n} \sum_{i=1}^{n}$ for $n \ll N$,

$$\widetilde{\nabla F}(\beta) = \frac{1}{n} \sum_{i \in I_n} \nabla \textbf{Loss}(\beta, x_i, y_i) \; + \; \nabla \Omega(\beta)$$

where I_n is a (random) subset with n elements.

Stochastic Gradient descent (SGD)

- For a learning rate $\eta > 0$ the SGD algorithm is as follows,

$$x_{n+1} = x_n - \eta \widetilde{\nabla F}(x_n)$$