UNIVERSITY AT ALBANY
STATE UNIVERSITY OF NEW YORK

CSI 436/536 (Fall 2024)

Machine Learning

Lecture 3: Review of Calculus and Optimization

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Announcement

- Course project list will be released later today on Gradescope!
  - Enroll in Gradescope ASAP if you haven't done yet
  - Your group chooses to work on one of them, or
  - Your group chooses to work a project beyond this list
    - You need my approval
    - You may come to my office hour to discuss it
- Participation points are given starting today!
  - Come to me to claim 1 point after this lecture, if
    - You asked a question, or
    - You showed/explained your solutions to in-class exercise problems

Recap: linear algebra review

- Vector:
  - Norm (one vector):
    - l_p norm (l_1, l_2, l_∞)
  - Distance and angle (two vectors)
  - Linear (in)dependence
  - Orthogonality: $x^\mathrm{T} y = 0$
- Matrix:
  - Matrix-vector multiplication, matrix-matrix multiplication
  - Rank, trace, determinant, symmetric, invertible
  - Eigenvalues and eigenvectors

Recap: positive (semi)-definite matrix

Very important property for optimization, kernel methods

- A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is positive semi-definite, if and only if $x^T A x \geq 0$, for any $x \in \mathbb{R}^n$.
  - All eigenvalues of A are non-negative.
  - $X^T A X$ for any $X \in \mathbb{R}^{n \times m}$ is positive semi-definite.
- A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is positive definite, if and only if $x^T A x > 0$, for any $0 \neq x \in \mathbb{R}^n$.
  - All eigenvalues of A are positive.
  - All diagonal entries of A are positive.

In class exercise: prove $A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$ is a positive definite matrix

- Solution 1: prove $x^T Ax \geq 0$ for any vector x.

- Solution 2: prove all eigenvalues of A are all non-negative.
  - Hint: solve $\det(A - \lambda I) = 0$ to find eigenvalues.

Today's agenda

- Multi-variate calculus
  - Partial derivative and gradient
  - Chain rule
  - Multiple integrals
  - Jacobian matrix and Hessian matrix
- Optimization
  - Convex set and convex function
  - Optimization problem formulation
  - Properties of convex optimization
  - Lagrange Multipliers

Multi-variate function

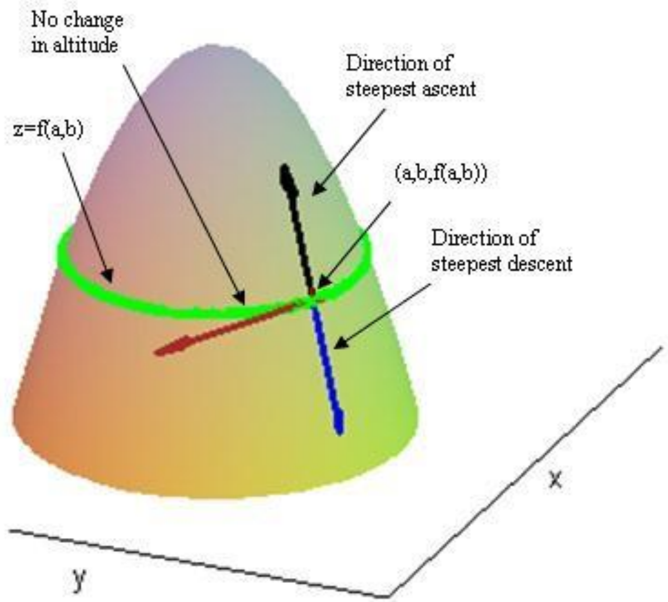
- Definition:
  - A function of two or more variables takes multiple inputs and produces a single output.
  - Examples: $f(x, y) = e^{x+y} + e^{3xy} + e^{y^4}$
- Domain:
  - Set of all possible inputs
- Range:
  - Set of possible output values.

Partial derivative

- Definition:
  - The rate of change of a function with respect to one variable, holding other variables constant.
- Notations:
  - $\frac{\partial f}{\partial x}$ or $\nabla_x f(x, y)$
- Example:
  - $f(x, y) = e^{x+y} + e^{3xy} + e^{y^4}$
    - $\frac{\partial f}{\partial x} = e^{x+y} + 3ye^{3xy}$
    - $\frac{\partial f}{\partial y} = e^{x+y} + 3xe^{3xy} + 4y^3 e^{y^4}$

Gradient

- Definition:
  - A vector that points in the direction of the steepest change. It is composed of the partial derivatives of the function with respect to each variable:
  - Example of $f(x,y)$:
    - $\nabla f(x,y) = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)$
- Interpretation:
  - It indicates the direction and rate of fastest change of the function.



Chain rule

- To compute derivative of a composite function
- Example:
  - $z = f\big(g(t)\big)$
  - $\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{\mathrm{d}f}{dg}\frac{\mathrm{d}g}{\mathrm{d}t}$
- In-class exercise:
  - $f(x) = e^{2x}, g(x) = \sin(x)$. Find $\nabla f(g(x))$.
  - $\frac{\mathrm{d}f}{dg} = 2e^{2g(x)} = 2e^{2\sin(x)}$
  - $\frac{\mathrm{d}z}{\mathrm{d}t} = \frac{\mathrm{d}f}{dg}\frac{\mathrm{d}g}{\mathrm{d}t} = 2e^{2\sin(x)}\cos(x)$

Multiple Integrals

- Double integral: compute the volume under a surface in two dimensions.
- Example: a function $f(x, y)$ over a region R
  - $\iint_R f(x, y)\, dx\, dy$
- In-class exercise: find double integral of the function $f(x, y) = x^2 + y^2$ over $0 \leq x \leq 2$ and $1 \leq y \leq 3$.
  - $\int_0^2 x^2\, dx = 8/3$
  - $\int_0^2 y^2\, dx = 2y^2$
  - $\int_1^3 \left(\frac{8}{3} + 2y^2\right) dy = 16/3 + 52/3 = \ 68/3$

Jacobian matrix – first order

$$\mathbf{J}_{ij} = \frac{\partial f_i}{\partial x_j}$$

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^{\mathrm{T}} f_1 \\ \vdots \\ \nabla^{\mathrm{T}} f_m \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}$$

- In-class exercise:
  - $f(x, y) = (f_1, f_2, f_3)$
  - $f_1 = x^2 y, f_2 = y^3, f_3 = 4xy + 5$

$$J_{3x2} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x} & \dfrac{\partial f_1}{\partial y} \\ \dfrac{\partial f_2}{\partial x} & \dfrac{\partial f_2}{\partial y} \\ \dfrac{\partial f_3}{\partial x} & \dfrac{\partial f_3}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy & x^2 \\ 0 & 3y^2 \\ 4y & 4x \end{bmatrix}$$

Hessian matrix – second order

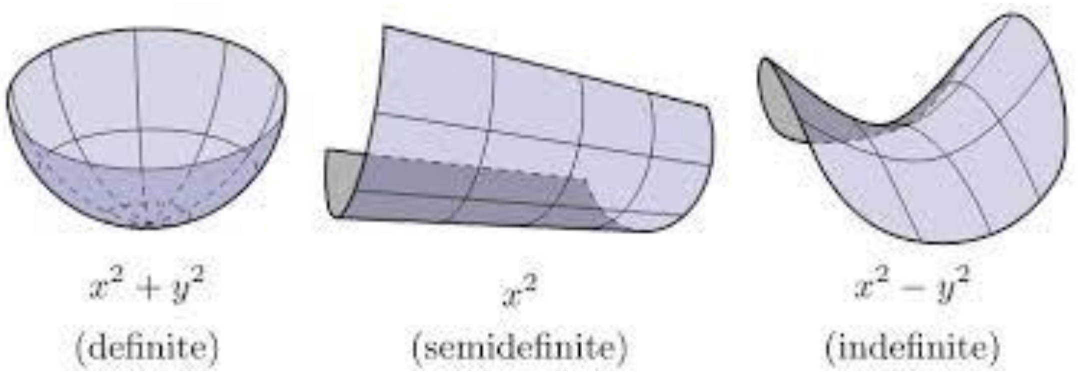
$$(\mathbf{H}_f)_{i,j} = \frac{\partial^2 f}{\partial x_i \, \partial x_j}$$

$$\mathbf{H}_f = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \, \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1 \, \partial x_n} \\[2.2ex] \dfrac{\partial^2 f}{\partial x_2 \, \partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2 \, \partial x_n} \\[2.2ex] \vdots & \vdots & \ddots & \vdots \\[2.2ex] \dfrac{\partial^2 f}{\partial x_n \, \partial x_1} & \dfrac{\partial^2 f}{\partial x_n \, \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

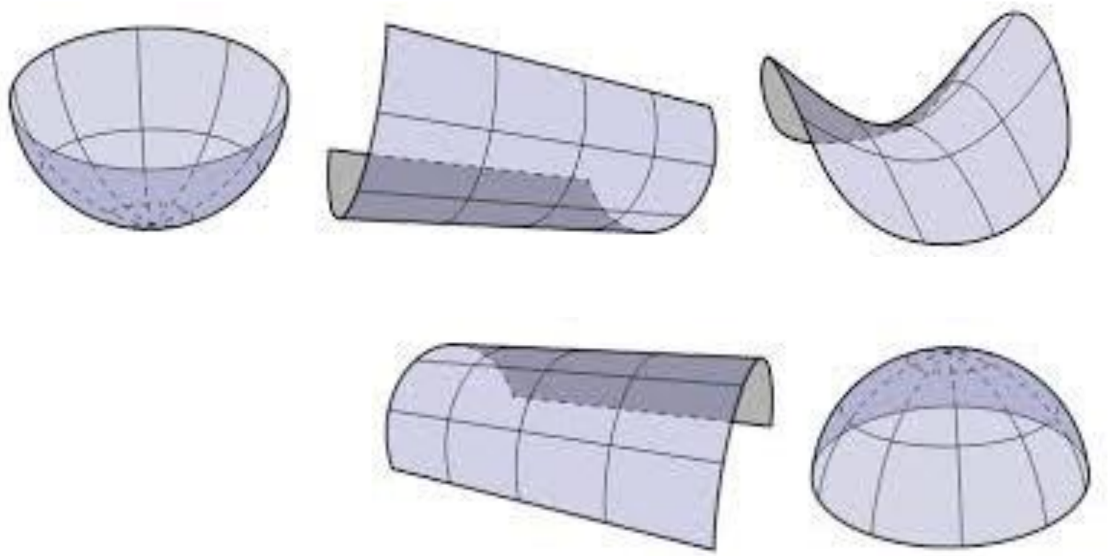
- Quadratic approximation of a function
  - $f(x+y) = f(x) + y^T \nabla f(x) + ½ y^T \nabla^2 f(x) y$

Hessian matrix – second order

- Hessian matrix is symmetric
- Hessian matrix and local curvature of the function
  - Minimum: Hessian is positive definite
  - Maximum: Hessian is negative definite
  - Saddle point: Hessian is indefinite (not positive/negative definite)



Quadratic Function



- $f(x) = \frac{1}{2}x^T Ax + b^T x + c$
  - Gradient: $\nabla f(x) = Ax + \mathrm{b}$
  - Hessian: $\nabla^2 f(x) = A$
- Quadratic programming:
  - $min\ f(x) = \frac{1}{2}x^T Ax + b^T x + c$
  - Key: check Hessian matrix!
    - Hessian is positive (semi)definite: minimum (local or global)
    - Hessian is negative (semi)definite: maximum (local or global)
    - Hessian is indefinite: undetermined, changing curvature
- Semi-definiteness determines uniqueness of solution

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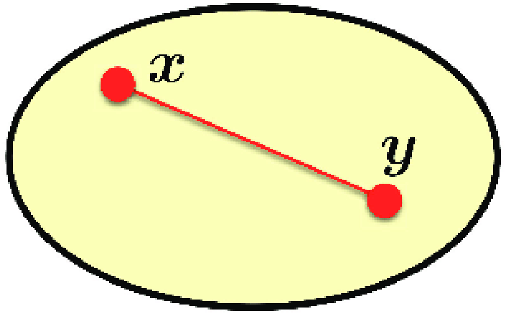
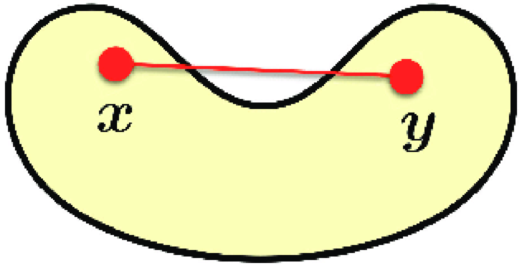
  - Convex set and convex function
  - Optimization problem formulation
  - Properties of convex optimization
  - Lagrange Multipliers

Convex Sets

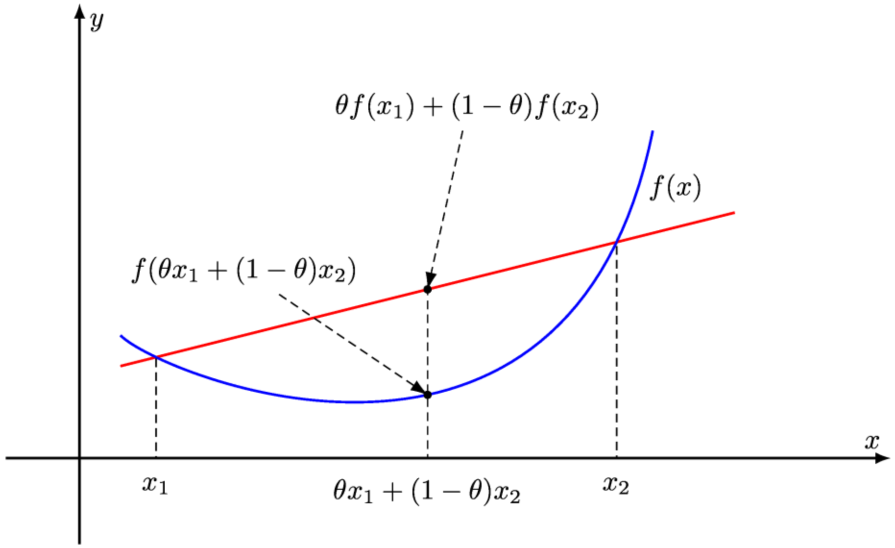
- Definition:
  - A set $C \subseteq R^n$ is convex if for any two points $x_1, x_2 \in C, \theta x_1 + (1-\theta)x_2 \in C$ for all $\theta \in [0,1]$.
- Interpretation:
  - A set $C \subseteq R^n$ is convex if, for any two points $x_1, x_2 \in C$, the line segment connecting them is also entirely within C.
- Discussion: are they convex sets?
  - (1) [0,1]
  - (2-3)





Convex functions

- Definition:
  - A function $f: C \rightarrow R$ is convex if C is a convex set and for all $x_1, x_2 \in C$ and $\theta \in [0,1]$:
  - $f(\theta x_1 + (1-\theta)x_2) \leq \theta f(x_1) + (1-\theta)f(x_2)$
- Interpretation:
  - A convex function lies below the line segment connecting any two points on its graph.
- Discussion: propose some convex functions
- Example: linear functions, quadratic functions, exponential functions.



Convex optimization problem formulation

- $\min f(x)$,
- $\mathrm{s.t.}\ \mathrm{g}(x) \leq 0, h(x) = 0$.

- $f(x)$ is the convex objective function
- $g(x)$ is convex inequality constraint
- h(x) is equality constraint

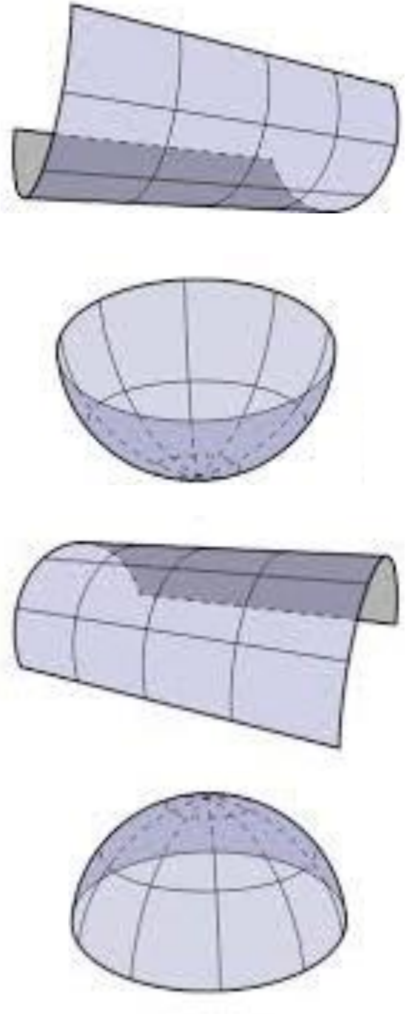
Review of 1-dimensional optimization

- $f(x) = x^3 + 3x^2 - 24x + 2$

  - First, solve $f'(x) = 0$ to get all solutions $f'(x) = 3x^2 + 6x - 24 = 0, x_1 = -4, x_2 = 2.$
  - Second, for each solution, check $f''(x)$: $f''(x) = 6x + 6$
    - $f''(x) > 0$: minimum (local or global) $x = 2$
    - $f''(x) < 0$: maximum (local or global) $x = -4$
    - $f''(x) = 0$: undetermined, changing curvature

Hessian matrix and convex function

- $\nabla^2 f(x) \succcurlyeq 0$, then f(x) is convex
  - No local minimum
- $\nabla^2 f(x) \succ 0$, then f(x) is strongly convex
  - Unique global minimum
- $-\nabla^2 f(x) \succcurlyeq 0$, then f(x) is concave
  - No local maximum
- $-\nabla^2 f(x) \succ 0$, then f(x) is strongly concave
  - Unique global maximum



Properties of convex optimization problems

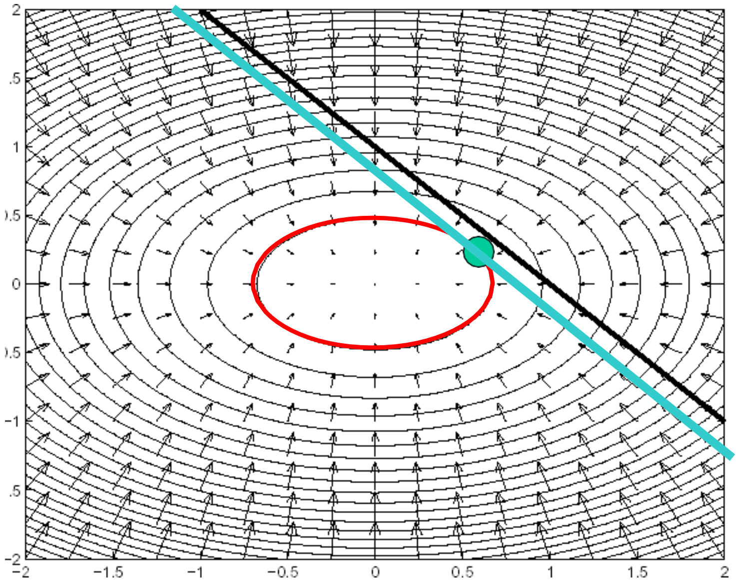
- **Global Optimum**: A convex optimization problem has no local minima other than the global minimum. If a solution is found, it is guaranteed to be optimal.
- **Duality**: Convex optimization problems have associated dual problems that provide bounds on the solution. The **Lagrange dual function** plays a crucial role in this.
- **Strong Duality**: In many convex problems (e.g., if the Slater's condition holds), the optimal value of the primal problem equals the optimal value of the dual problem.

Lagrange multipliers to handle constraints

- The Lagrangian function combines the objective function with the constraints using multipliers.
- Example: $\max xy, \text{s.t.}\ x + y = c$
  - Solution 1: use $y = c - x$, then objective problem is $\max x(c - x)$, so $x = y = c/2$ is the optimal solution.
  - Solution 2 (Lagrange multiplier):
    - $L(x, y, \lambda) = xy - \lambda(x + y - c)$
    - Differentiate with regards to x and y, we have $x = y = \lambda$
  - Note xy is neither convex or concave, so only with constraint it has a solution

Equality constrained problem

- $\min f(x, y) = x^2 + 2y^2 - 2$
- s.t. $x + y = 1$



Equality constrained problem

- $\min f(x, y) = x^2 + 2y^2 - 2$
- s.t. $x + y = 1$

Introduce Lagrangian multiplier λ and form

- Solution:

$$L(x, y, \lambda) = x^2 + 2y^2 - 2 \;\; - \lambda(x + y - 1)$$

Then, differentiate with respect to x, y, λ : and set derivative to 0.

$$\left.\begin{aligned}
\frac{\partial L}{\partial x} &= 2x - \lambda = 0 &&\Rightarrow \quad \lambda = 2x \\
\frac{\partial L}{\partial y} &= 2y - \lambda = 0 &&\Rightarrow \quad \lambda = 4y \\
\frac{\partial L}{\partial \lambda} &= -x - y + 1 = 0 &&\Rightarrow \quad -x - y + 1 = 0
\end{aligned}\right\} \quad
\begin{aligned}
\lambda &= \frac{4}{3} \\
x &= \frac{2}{3} \\
y &= \frac{1}{3}
\end{aligned}$$

Equality constrained problem in matrix

- $min_x f(x) = \frac{1}{2} x^T A x + b^T x + c, s.t. Dx = e$
    - Introduce Lagrangian multiplier **v** and form Lagrangian $L(x, v) = f(x) - v^{\mathsf{T}}(Dx - e)$
    - Optimal solution given at the stationary point of L

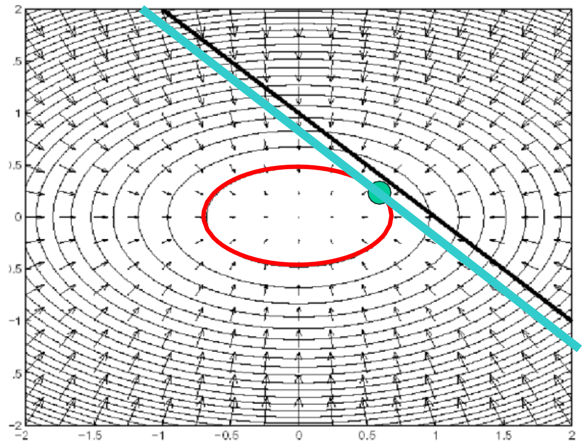
      $$\frac{\partial L}{x} = b + Ax - D^T v = 0 \quad \text{(dual feasibility)}$$

      $$\frac{\partial L}{\partial v} = Dx - e = 0 \quad \text{(primal feasibility)}$$

    - Solution: solving the KKT equation

      $$\begin{pmatrix} A & -D^{\mathsf{T}} \\ D & 0 \end{pmatrix} \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} -b \\ e \end{pmatrix}$$

Previous example



Rewrite the problem: Let $x_1 = x, x_2 = y$

$$\min_{x_1,x_2} f(x_1,x_2) = {x_1}^2 + 2{x_2}^2 - 2, s.t.\ x + y = 1$$

$$f = (x_1, x_2)\begin{pmatrix}1 & 0\\ 0 & 2\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix} + \begin{pmatrix}0\\ 0\end{pmatrix}\begin{pmatrix}x_1\\ x_2\end{pmatrix} - 2$$

$$so, A = \begin{pmatrix}2 & 0\\ 0 & 4\end{pmatrix}, b = \begin{pmatrix}0\\ 0\end{pmatrix}, c{=}{-2}$$

$$(1,1)\begin{pmatrix}x_1\\ x_2\end{pmatrix} = e = 1$$

$$so, D = (1,1), e = 1$$

Solution given by $\begin{pmatrix}A & -D^\top\\ D & 0\end{pmatrix}\begin{pmatrix}x\\ v\end{pmatrix} = \begin{pmatrix}-b\\ e\end{pmatrix}$

That is, $\begin{pmatrix}2 & 0 & -1\\ 0 & 4 & -1\\ 1 & 1 & 0\end{pmatrix}\begin{pmatrix}x\\ y\\ v\end{pmatrix} = \begin{pmatrix}0\\ 0\\ 1\end{pmatrix}$

In-class exercise

- Find maximum and minimum values of the function
  - $f(x, y, z) = x^2 + y^2 + z^2$
  - subject to the constraint $g(x, y, z) = x^2 + y^2 - z = 1$.