Math Basics for DS

Practical Session 9

Today

- Short quiz univariate calculus
- Multivariate calculus

Quiz

- https://forms.gle/hV6QkGjuC8RZgRMp6

Partial Derivatives

- Derivative for univariate functions:

$$y = f(x), \qquad \frac{dy}{dx} = f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

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- **Partial derivative** for multivariate functions:

$$y = f(x_1, \dots, x_n), \qquad \frac{\partial y}{\partial x_i} = f'_{x_i} = \lim_{\Delta x \to 0} \frac{f(x_1, \dots, x_i + \Delta x_i, \dots, x_n) - f(x_1, \dots, x_i, \dots x_n)}{\Delta x_i}$$

Compute derivative with respect to x_i
regarding all other variables as constants.

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Partial Derivatives - Example

- Let $f(x, y) = x^3 + x^2y^3 - 2y^2$.

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$$f_y(x, y) = \frac{\partial f}{\partial y} = 3x^2y^2 - 4y \Big|_{(2,1)} = 12 - 4 = 8$$

The Chain Rule

- For univariate functions:

$$\left(f\left(g(x)\right)\right)' = f'\left(g(x)\right) \cdot g'(x) \quad \Leftrightarrow \quad \frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}$$

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- For multivariate functions:

$$u(x_1, \dots, x_n), \qquad x_i = x_i(t_1, \dots, t_m)$$

$$\frac{\partial u}{\partial t_k} = \frac{\partial u}{\partial x_1} \cdot \frac{\partial x_1}{\partial t_k} + \frac{\partial u}{\partial x_2} \cdot \frac{\partial x_2}{\partial t_k} + \cdots + \frac{\partial u}{\partial x_n} \cdot \frac{\partial x_n}{\partial t_k}, \qquad k = 1, \dots, m$$

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$$\frac{\partial u}{\partial t} = (2xy + 3y^4) \cdot 2\cos 2t + (x^2 + 12xy^3)(-\sin t)$$

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$$u = x^4 y + y^2 z^3$$

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$$\frac{\partial u}{\partial s} = 4x^3 y \cdot re^t + (x^4 + 2yz^3) \cdot 2rse^{-t} + 3y^2 z^2 \cdot r^2 \sin t$$

Gradient

- A vector of partial derivatives:

$$\nabla f(x_1, \dots, x_n) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right)$$

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- Example:

$$f(x, y, z) = e^{xy} \ln z$$

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Gradient

Gradient shows the direction of the maximal growth of the function.

Negative gradient = direction of the maximal descent of the function.

Higher Derivatives

- Consider $f(x, y)$.
- $f'_x(x, y),\ f'_y(x, y)$ – also functions of two variables.
  We can compute their partial derivatives!

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- $f'_x(x, y),\ f'_y(x, y)$ – also functions of two variables.
  We can compute their partial derivatives!

$$(f'_x)'_x = f''_{xx}(x, y) = \frac{\partial^2 f}{\partial x^2}, \qquad (f'_x)'_y = f''_{xy}(x, y) = \frac{\partial^2 f}{\partial y \partial x}$$

$$\left(f'_y\right)'_y = f''_{yy}(x, y) = \frac{\partial^2 f}{\partial y^2}, \qquad \left(f'_y\right)'_x = f''_{yx}(x, y) = \frac{\partial^2 f}{\partial x \partial y}$$

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Higher Derivatives - Example

- Consider $f(x,y) = x^3 + x^2y^3 - 2y^2$.

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$$f''_{xx}(x,y) = \frac{\partial^2 f}{\partial x^2} = 6x + 2y^3, \qquad f''_{xy}(x,y) = \frac{\partial^2 f}{\partial y \partial x} =$$

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Hessian

- A matrix of second derivatives.
- $f(x_1, \dots, x_n)$

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_2 x_1} & \cdots & \frac{\partial^2 f}{\partial x_n x_1} \\ \frac{\partial^2 f}{\partial x_1 x_2} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n x_1} & \frac{\partial^2 f}{\partial x_n x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

Hessian - Example

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$$H = \begin{pmatrix} 6x + 2y^3 & 6x \\ 6x & 6x^2y - 4 \end{pmatrix}$$

Extrema

- Univariate case: a stationary point x_0 is a local minimum (maximum) if

$$f''(x_0) > 0 \ (f''(x_0) < 0).$$

- Multivariate case:

x_0 is a stationary point: $\nabla f(x_0) = 0$

$H -$ Hessian.

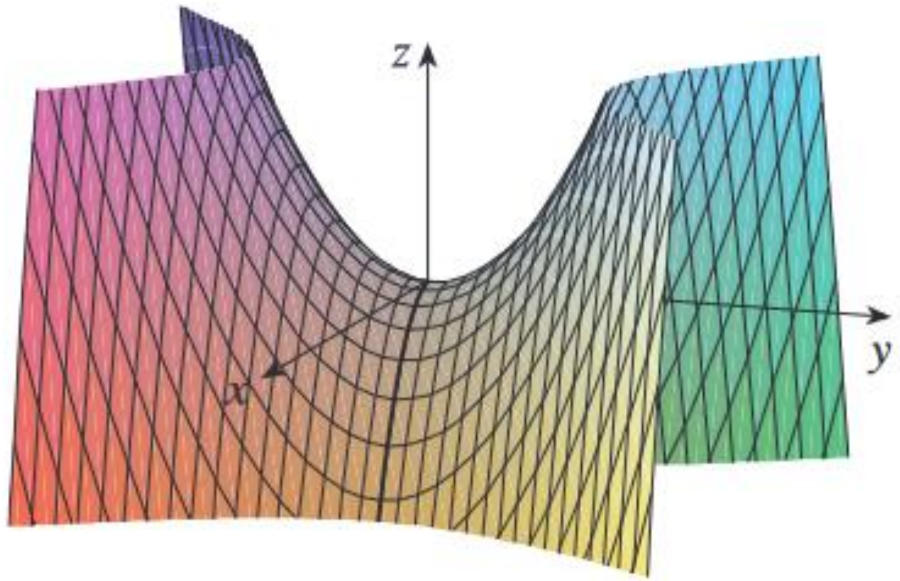
Then, if H is a **positive-definite** matrix, then x_0 is a **local minimum**.

If H is a **negative-definite** matrix, then x_0 is a **local maximum**.

If $\det H = 0$, we need to check manually.

Otherwise, x_0 is a **saddle point**.

Saddle Points



Positive vs Negative Definite Matrices

- A matrix A is called positive-definite if

$$x^T A x > 0 \ \forall x$$

- A matrix A is called negative-definite if

$$x^T A x < 0 \ \forall x$$

Positive vs Negative Definite Matrices

- How to check if a matrix is positive (negative) definite?

Positive vs Negative Definite Matrices

- How to check if a matrix is positive (negative) definite?

  Check principal minors D_k!

For positive definite:

$$D_1 > 0, \quad D_2 > 0, \quad \ldots, D_n > 0$$

For negative definite:

$$D_1 < 0, \quad D_2 > 0, \quad D_3 < 0, \ldots$$

$$H = \begin{pmatrix} \boxed{\dfrac{\partial^2 f}{\partial x_1^2}} & \dfrac{\partial^2 f}{\partial x_2 x_1} & \cdots & \dfrac{\partial^2 f}{\partial x_n x_1} \\ \dfrac{\partial^2 f}{\partial x_1 x_2} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2 x_n} \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial^2 f}{\partial x_n x_1} & \dfrac{\partial^2 f}{\partial x_n x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

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$$f(x, y) = x^4 + y^4 - 4xy + 1$$

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Stationary points: $\nabla f = 0 \quad \Leftrightarrow$

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Stationary points: $\nabla f = 0 \quad \Leftrightarrow$

$$\begin{aligned} 4x^3 - 4y &= 0 \\ 4y^3 - 4x &= 0 \end{aligned} \quad \Leftrightarrow$$

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$$\begin{matrix} 4x^3 - 4y = 0 \\ 4y^3 - 4x = 0 \end{matrix} \quad \Longleftrightarrow \quad \begin{matrix} y = x^3 \\ x^9 - x = 0 \end{matrix} \quad \Longleftrightarrow$$

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Stationary points: $(0,0),\ (-1,-1),\ (1,1)$

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$$H = \left(\qquad\qquad \right)$$

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$$H = \begin{pmatrix} 12x^2 & -4 \\ -4 & 12y^2 \end{pmatrix}$$

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$\det H = 144x^2y^2 - 16|_{(0;0)} < 0,\ (0,0)$ – saddle point.

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$$H = \begin{pmatrix} 12x^2 & -4 \\ -4 & 12y^2 \end{pmatrix}$$

$$\det H = 144x^2y^2 - 16 \Big|_{(1;1)} > 0, \qquad \det H_1 = 12x^2 \Big|_{(1,1)} > 0$$

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$(1, 1)$ – local minimum.

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Stationary points: $(0, 0)$, $(-1, -1)$, $(1, 1)$

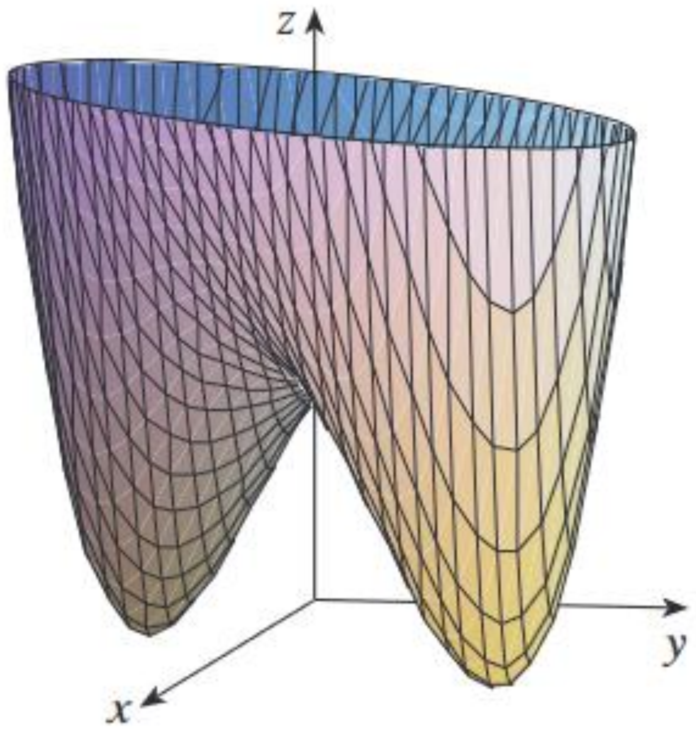
$$H = \begin{pmatrix} 12x^2 & -4 \\ -4 & 12y^2 \end{pmatrix}$$

$$\det H = 144x^2y^2 - 16 \Big|_{(-1;-1)} > 0, \qquad \det H_1 = 12x^2 \Big|_{(-1,-1)} > 0$$

$(-1, -1)$ – local minimum.

Extrema – Example

$$f(x, y) = x^4 + y^4 - 4xy + 1$$



Linear Regression the Other Way

Least Squares (Again)

- Remember the Least Squares problem:

$$\hat{y}_i = w_0 + w_1 x_1^i + \cdots + w_n x_n^i, \qquad y_i = \hat{y}_i + e_i, \qquad w = ?$$

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$$\hat{w} = (X^T X)^{-1} X^T y$$

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- We can also see this as an optimization problem:

$$\mathcal{L}(w_0, \dots, w_n) = \sum e_i^2 = \sum (y_i - \hat{y})^2 = \sum \left(y_i - \left(w_0 + w_1 x_1^i + \cdots + w_n x_n^i\right)\right)^2 \to \min_{w_0, \dots, w_n}$$

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Least Squares

- Let's consider a simple case: fitting a line to a set of points

$$(x_1, y_1), \qquad (x_2, y_2), \qquad \dots, \qquad (x_n, y_n)$$

$$y \approx w_0 + w_1 x$$

We want to pick the weights $w_0,\ w_1$
so that the sum of squares of the errors is the smallest possible:

$$\mathcal{L}(w_0, w_1) = \qquad \qquad \rightarrow \min_{w_0, w_1}$$

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Least Squares

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Least Squares

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Least Squares

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$$\frac{\partial \mathcal{L}}{\partial w_1} = \sum_{i=1}^{n} x_i y_i - w_0 \sum_{i=1}^{n} x_i - w_1 \sum_{i=1}^{n} x_i^2 = 0$$

$$\frac{\partial \mathcal{L}}{\partial w_0} = \sum_{i=1}^{n} y_i - w_1 \sum_{i=1}^{n} x_i - n w_0 = 0$$

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Least Squares

$$\mathcal{L}(w_0, w_1) = \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \to \min_{w_0, w_1}$$

$$w_0 \sum_{i=1}^{n} x_i + w_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

$$n w_0 + w_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

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Least Squares

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$$w_0 \sum_{i=1}^{n} x_i + w_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i y_i$$

$$w_0 + w_1 \frac{1}{n} \sum_{i=1}^{n} x_i = \frac{1}{n} \sum_{i=1}^{n} y_i \quad \Leftrightarrow \quad w_0 + w_1 \bar{x} = \bar{y}$$

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Least Squares

$$\mathcal{L}(w_0, w_1) = \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \rightarrow \min_{w_0, w_1}$$

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$$n w_0 + w_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$

$$w_0 + w_1 \bar{x} = \bar{y}$$

Least Squares

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$$w_0 + w_1 \bar{x} = \bar{y}$$

$$n w_0 \sum_{i=1}^{n} x_i + w_1 \left(\sum_{i=1}^{n} x_i \right)^2 = \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i$$

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Least Squares

$$\mathcal{L}(w_0, w_1) = \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \to \min_{w_0, w_1}$$

$$w_1 \left(\sum_{i=1}^{n} x_i \right)^2 - n w_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i - n \sum_{i=1}^{n} x_i y_i$$

$$w_1 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i \right)^2}$$

Least Squares

$$\mathcal{L}(w_0, w_1) = \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2 \to \min_{w_0, w_1}$$

$$\widehat{w}_0 = \widehat{w}_1 \bar{x} = \bar{y},$$

$$\widehat{w}_1 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$