Introduction to intelligent systems

Optimization

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Overview

1. Gradient descent
2. Linear regression (with gradient descent)
3. Neural network (with gradient descent)
4. Tasks

Feedback group

- Nicholas Borch
- Alfred Fonnesbech Aqraou
- Josefine Høgsted Voglhofer
- Rasmus Bernth Linnemann

Learning objectives

- II Gradient descent algorithm.
- I Stochastic gradient descent.
- II Gradient of cost function.
- II Neural networks: Model (layers, activation functions), parameters, cost function.

- I Understand the concepts and definitions, and know their application. Reason about the concepts in the context of an example. Use correct technical terminology.
- II As above plus: Read, manipulate, and work with technical definitions and expressions (mathematical and Python code). Carry out practical computations. Interpret and evaluate results.

Gradient descent

Gradient descent

- Iterative method for finding optimum of a function
- Start at an initial point
- Updates parameters by taking step proportional to negative of the gradient
- Repeat until convergence

Partial derivative

- Derivative of a function of *several variable* with respect to *one* of those variables, with the others *held constant*.
- Notation

$$\frac{\partial f}{\partial x_1}, \qquad \frac{\partial f(x_1, x_2)}{\partial x_1}, \qquad \frac{\partial f}{\partial x_1}(x_1, x_2)$$

- The partial derivative evaluated at a certain point

$$\left.\frac{\partial f}{\partial x_1}\right|_{x_1=5, x_2=7}$$

Partial derivative, definition

Derivative, function of single variable, $f(x)$

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Partial derivative, definition

Derivative, function of single variable, $f(x)$

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

Partial derivative, function of multiple variables, $f(x_1, x_2)$

$$\frac{\partial f}{\partial x_1}(x_1, x_2) = \lim_{h\to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

Partial derivative, definition

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$$\frac{\partial f}{\partial x_2}(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1, x_2 + h) - f(x_1, x_2)}{h}$$

Gradient

Definition

$$\nabla f(x_1, x_2, \dots) = \begin{bmatrix} \dfrac{\partial f(x_1, x_2, \dots)}{\partial x_1} \\[2ex] \dfrac{\partial f(x_1, x_2, \dots)}{\partial x_2} \\[2ex] \vdots \end{bmatrix}$$

Exercise: Gradient calculation

Multivariate function

$$f(x, y) = x^2 \cos(y)$$

What is the gradient?

Gradient definition

$$\nabla f(x, y) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} \\ \\ \dfrac{\partial f(x, y)}{\partial y} \end{bmatrix}$$

Exercise: Gradient calculation

Multivariate function

$$f(x, y) = x^2 \cos(y)$$

What is the gradient?

Partial derivatives

$$\frac{\partial f(x, y)}{\partial x} = 2x \cos(y)$$
$$\frac{\partial f(x, y)}{\partial y} = -x^2 \sin(y)$$

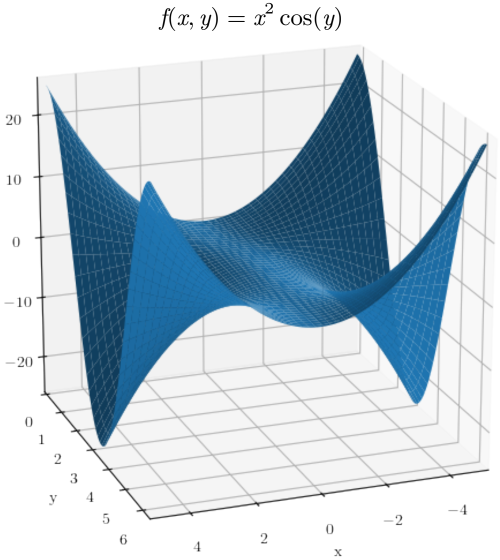
Gradient

$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x \cos(y) \\ -x^2 \sin(y) \end{bmatrix}$$

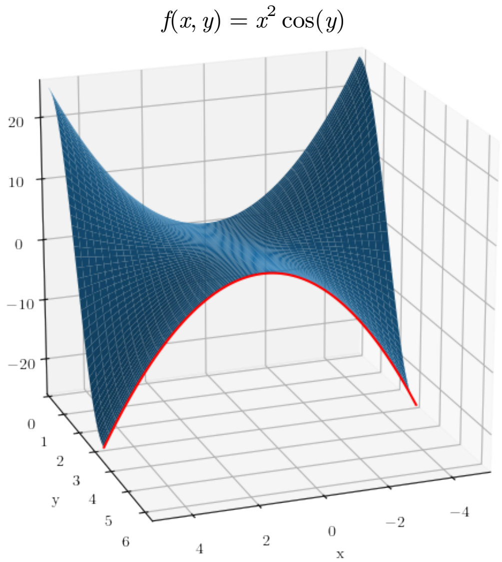
Gradient definition

$$\nabla f(x, y) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} \\ \\ \dfrac{\partial f(x, y)}{\partial y} \end{bmatrix}$$

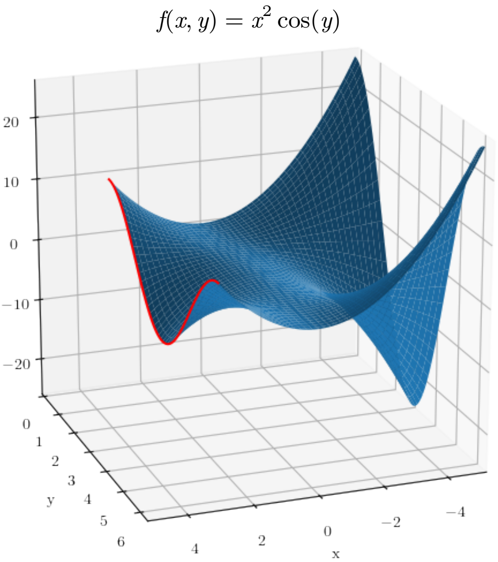
Gradient



Gradient



Gradient



Gradient descent

Initialize $x^{(0)}$
Repeat, $t = 0, 1, 2, \ldots$

$$\underbrace{x^{(t+1)}}_{\text{new parameter value}} = \underbrace{x^{(t)}}_{\text{old parameter value}} - \underbrace{\alpha}_{\text{step size}} \cdot \underbrace{\nabla f(x^{(t)})}_{\text{gradient}}$$

until convergence

Partial derivative in vector form

Partial derivative, function of multiple variables, $f(x_1, x_2)$

$$\frac{\partial f}{\partial x_1}(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$
$$\frac{\partial f}{\partial x_2}(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1, x_2 + h) - f(x_1, x_2)}{h}$$

Partial derivative in vector form

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$$\frac{\partial f}{\partial x_2}(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1, x_2 + h) - f(x_1, x_2)}{h}$$

Partial derivative in vector form, function of a vector, $f(\bar{x})$, where $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$$\frac{\partial f}{\partial x_1}(\bar{x}) = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{e}_1) - f(\bar{x})}{h}$$
$$\frac{\partial f}{\partial x_2}(\bar{x}) = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{e}_2) - f(\bar{x})}{h}$$

$$\bar{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \bar{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Directional derivative

How much does the function change if we move the parameters $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in the direction $\bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$

Directional derivative

How much does the function change if we move the parameters $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in the direction $\bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h}$$

Directional derivative

How much does the function change if we move the parameters $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in the direction $\bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$

$$\begin{aligned} \nabla_{\bar{v}} f(\bar{x}) &= \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} \\ &= \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h} \end{aligned}$$

Directional derivative

How much does the function change if we move the parameters $\bar{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ in the direction $\bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$

$$\begin{aligned}
\nabla_{\bar{v}} f(\bar{x}) &= \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} \\
&= \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h} \\
&= \nabla f(\bar{x}) \cdot \bar{v} \qquad \leftarrow \text{We will show this}
\end{aligned}$$

Directional derivative: Proof

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h}, \quad \bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

Directional derivative: Proof

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$$g(h) = f(\underbrace{x_1 + h \cdot v_1}_{z_1(h)}, \underbrace{x_2 + h \cdot v_2}_{z_2(h)}) = f(\bar{x} + h\bar{v})$$

Directional derivative: Proof

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h}, \quad \bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

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$$\left.\frac{\mathrm{d}g}{\mathrm{d}h}\right|_{h=0} = \lim_{\epsilon \to 0} \frac{g(0 + \epsilon) - g(0)}{\epsilon}$$

Directional derivative: Proof

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h\to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} = \lim_{h\to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h}, \quad \bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

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Directional derivative: Proof

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h}, \qquad \bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$g(h) = f(\underbrace{x_1 + h \cdot v_1}_{z_1(h)}, \underbrace{x_2 + h \cdot v_2}_{z_2(h)}) = f(\bar{x} + h\bar{v})$$

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$$= \frac{\partial f}{\partial z_1}\frac{\partial z_1}{\partial h} + \frac{\partial f}{\partial z_2}\frac{\partial z_2}{\partial h}$$

Directional derivative: Proof

$$\nabla_{\bar{v}} f(\bar{x}) = \lim_{h \to 0} \frac{f(x_1 + h \cdot v_1, x_2 + h \cdot v_2) - f(x_1, x_2)}{h} = \lim_{h \to 0} \frac{f(\bar{x} + h\bar{v}) - f(\bar{x})}{h}, \quad \bar{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$g(h) = f(\underbrace{x_1 + h \cdot v_1}_{z_1(h)}, \underbrace{x_2 + h \cdot v_2}_{z_2(h)}) = f(\bar{x} + h\bar{v})$$

$$\begin{aligned} \left.\frac{\mathrm{d}g}{\mathrm{d}h}\right|_{h=0} &= \lim_{\epsilon \to 0} \frac{g(0 + \epsilon) - g(0)}{\epsilon} \\ &= \lim_{\epsilon \to 0} \frac{f(\bar{x} + \epsilon\bar{v}) - f(\bar{x})}{\epsilon} = \underline{\nabla_{\bar{v}} f(\bar{x})} \\ \\ &= \frac{\partial f}{\partial z_1}\frac{\partial z_1}{\partial h} + \frac{\partial f}{\partial z_2}\frac{\partial z_2}{\partial h} \\ &= \frac{\partial f}{\partial z_1} v_1 + \frac{\partial f}{\partial z_2} v_2 = \underline{\nabla f \cdot \bar{v}} \end{aligned}$$

Direction of steepest descent

Directional derivative

$$\nabla_{\bar{v}} f(\bar{x}) = \nabla f(\bar{x}) \cdot \bar{v}$$

- Measures how much the function changes when we move a bit in the direction $\bar{v}$

Direction of steepest descent

Directional derivative

$$\nabla_{\bar{v}} f(\bar{x}) = \nabla f(\bar{x}) \cdot \bar{v}$$

- Measures how much the function changes when we move a bit in the direction $\bar{v}$

Which direction maximizes the directional derivative?

Direction of steepest descent

Directional derivative

$$\nabla_{\bar{v}} f(\bar{x}) = \nabla f(\bar{x}) \cdot \bar{v}$$

- Measures how much the function changes when we move a bit in the direction $\bar{v}$

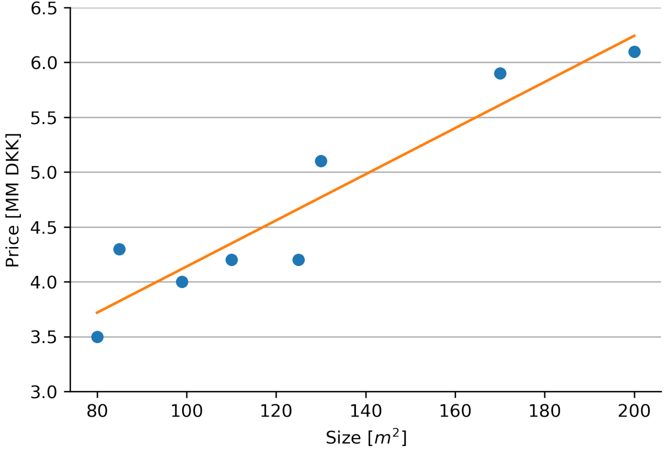
Which direction maximizes the directional derivative?
The dot product is maximal when the two vectors are parallel

$$\bar{v} = \frac{\nabla f(\bar{x})}{\|\nabla f(\bar{x})\|}$$

I.e. the gradient points in the direction of steepest ascent.

Linear regression (with gradient descent)

Remember linear regression



Gradient descent in linear regression

Linear regression

- Regression line: $f(x) = ax + b$
- Cost: Squared distance between data and regression line

$$E = \sum_{n=1}^{N} (y_n - f(x_n))^2$$

What is the gradient?

$$\nabla E(a, b) = \begin{bmatrix} \frac{\partial E(a,b)}{\partial a} \\ \frac{\partial E(a,b)}{\partial b} \end{bmatrix}$$

Gradient descent in linear regression

Linear regression

- Regression line: $f(x) = ax + b$
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$$E = \sum_{n=1}^{N} (y_n - f(x_n))^2$$

What is the gradient?

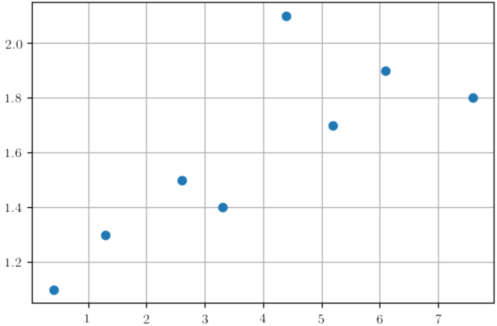
$$\nabla E(a, b) = \begin{bmatrix} \frac{\partial E(a,b)}{\partial a} \\ \frac{\partial E(a,b)}{\partial b} \end{bmatrix}$$

Solution

$$\frac{\partial E}{\partial a} = \sum_{n=1}^{N} -2(y_n - ax_n - b)x_n$$

$$\frac{\partial E}{\partial b} = \sum_{n=1}^{N} -2(y_n - ax_n - b)$$

Linear regression data

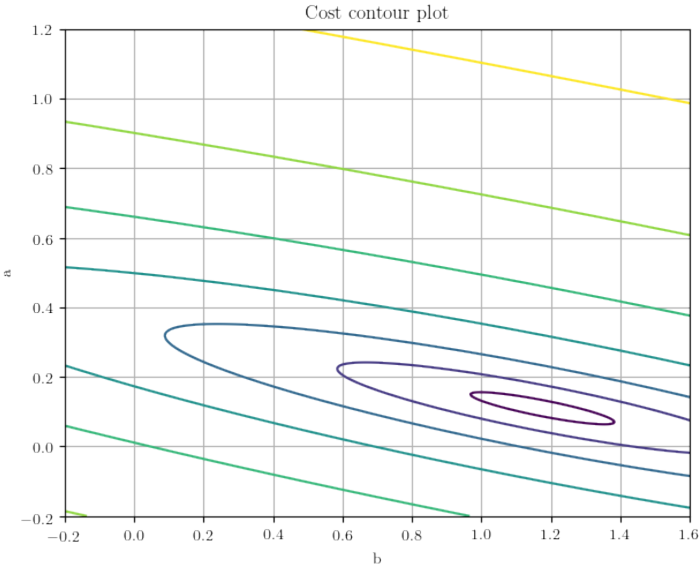


- Regression line: $f(x) = ax + b$
- Cost: Squared distance between data and regression line

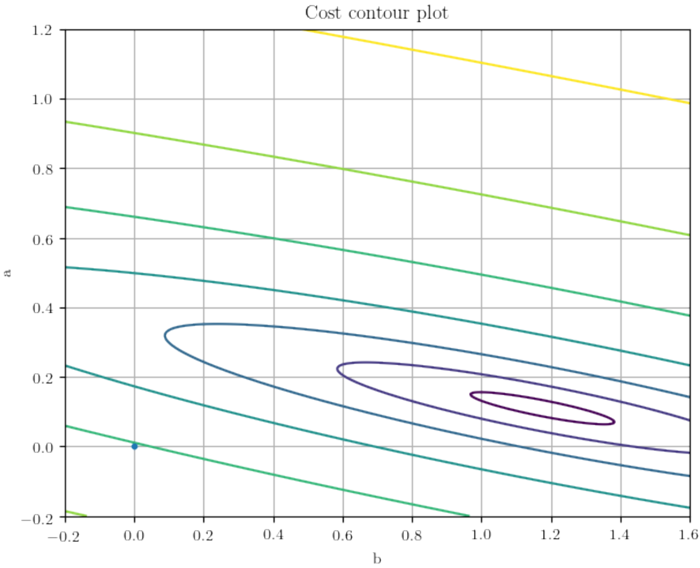
$$E = \sum_{n=1}^{N} (y_n - f(x_n))^2$$

The cost, $E(a, b)$, is a function of two variables. What does it look like?

Gradient steps



Gradient steps



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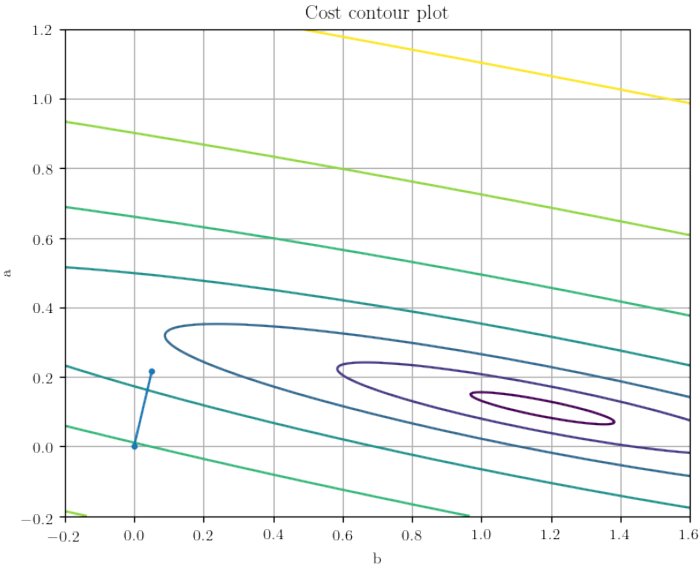
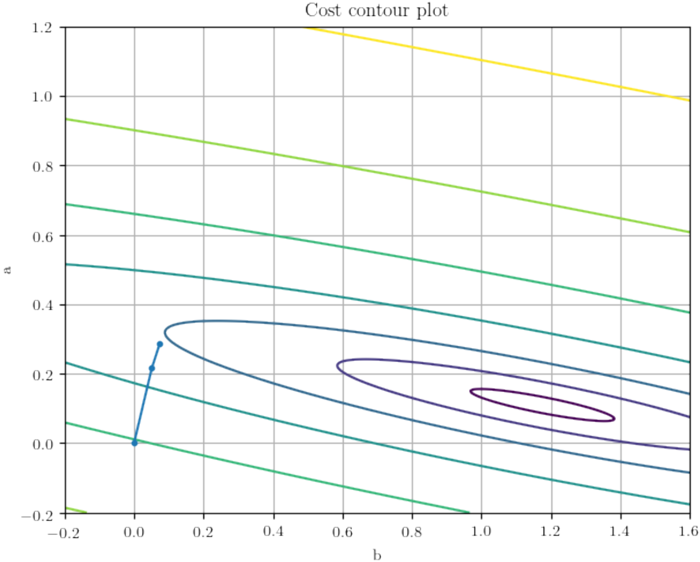
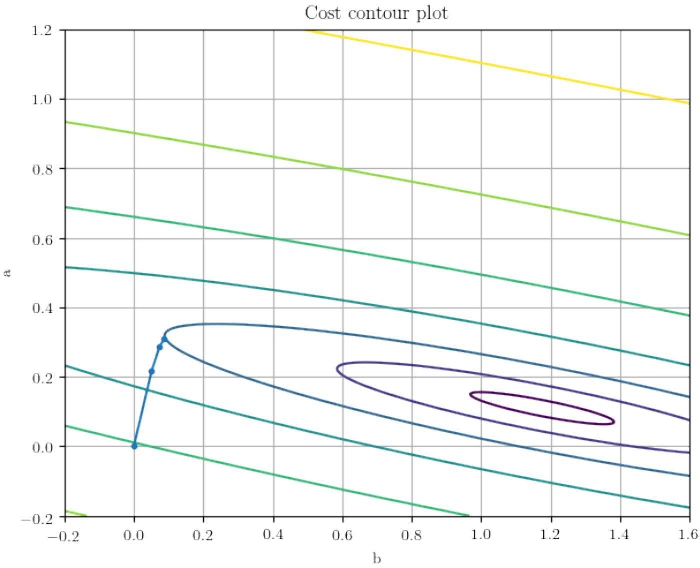


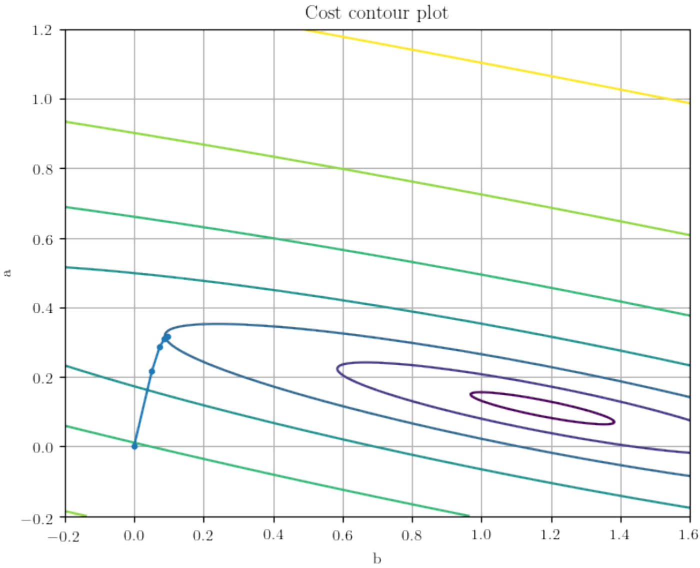
Gradient steps



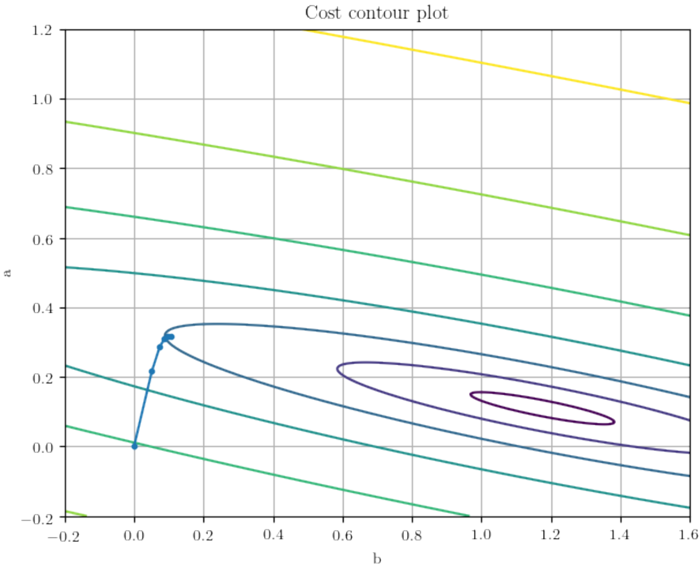
Gradient steps



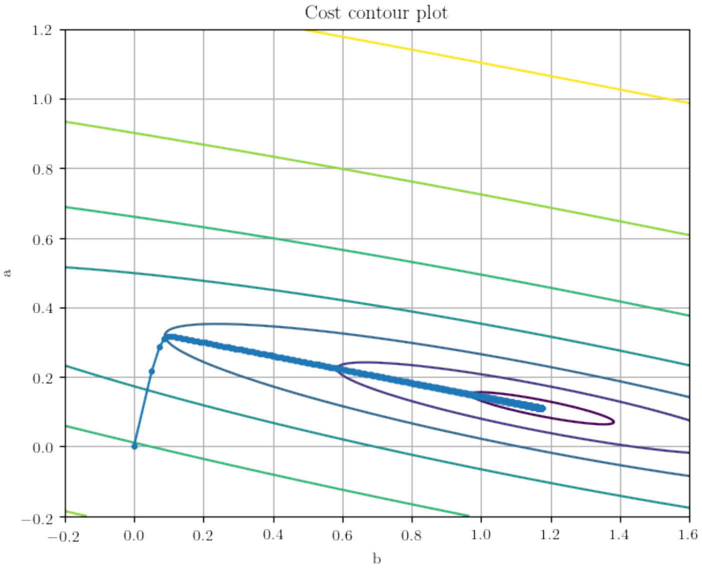
Gradient steps



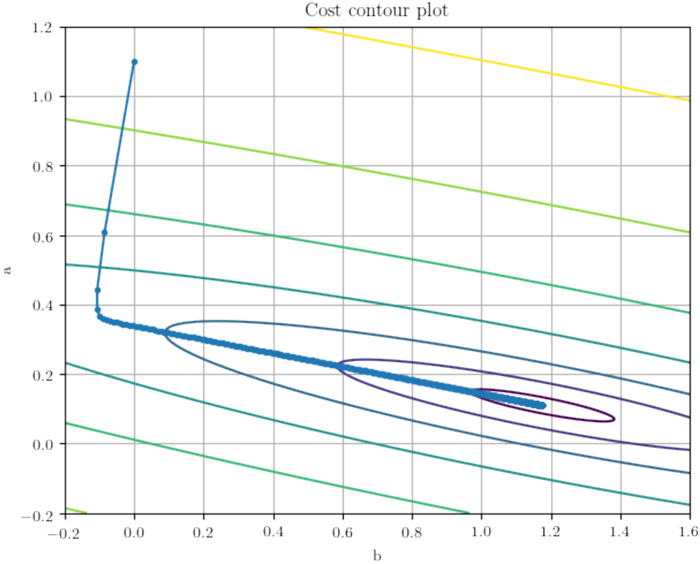
Gradient steps



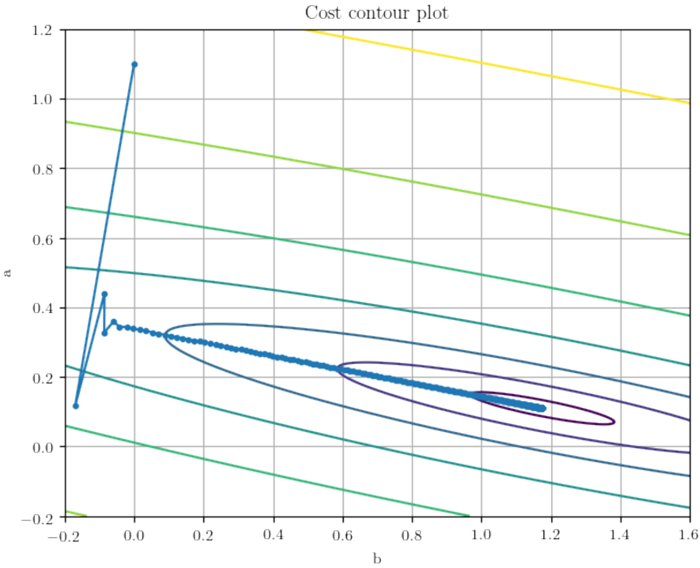
Gradient descent



Gradient descent



Gradient descent



Learning rate

- Small learning rate can lead to slow convergence
- Large learning rate may lead to divergence

Comparison with setting derivative equal to zero

Derivative equal to zero and solve

- No parameters to tune
- Closed form solution
- Slow for many features
  Need to solve N equations in N unknowns

Gradient descent

- Need to select step size
- Needs many iterations
- Fast for many features
  Need only compute the gradient

Feature scaling

- Is gradient descent sensitive to the scale of features? YES
- Features on different scale = parameters on different scale

Feature scaling

Min-max normalization

Rescale the range to $[0, 1]$

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Standardization

Rescale to have zero mean and unit variance

$$x' = \frac{x - \bar{x}}{\sigma_x}$$

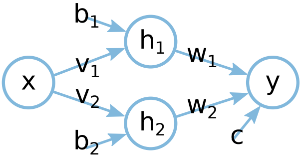
($\bar{x}$: mean, σ_x: standard deviation)

Neural network (with gradient descent)

Neural network

Cost function

$$E = \sum_{n=1}^{N} \left(y_n - \hat{y}_n\right)^2$$

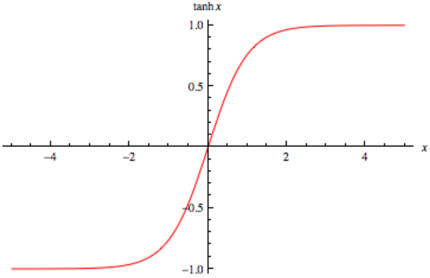


Network structure

$$\hat{y}_n = w_1 h_1(x_n) + w_2 h_2(x_n) + c$$

$$h_1(x_n) = \tanh\left(v_1 x_n + b_1\right)$$

$$h_2(x_n) = \tanh\left(v_2 x_n + b_2\right)$$



Model parameters

$$c,\ w_1,\ w_2,\ v_1,\ v_2,\ b_1,\ b_2$$

Exercise: Gradient of neural network

Compute the partial derivatives

$$\frac{\partial E}{\partial c}, \quad \frac{\partial E}{\partial w_1}, \quad \frac{\partial E}{\partial b_1}, \quad \frac{\partial E}{\partial v_1}$$

Hints

1. Use the chain rule
2. $\dfrac{\partial \tanh(x)}{\partial x} = 1 - \tanh^2(x)$
3. Don't expand terms needlessly. Express in terms of e.g. $\hat{y}_n$ and $h_1(x_n)$ where possible.

Cost function

$$E = \sum_{n=1}^{N} \left(y_n - \hat{y}_n\right)^2$$

Neural network model

$$\begin{aligned} \hat{y}_n &= w_1 h_1(x_n) + w_2 h_2(x_n) + c \\ h_1(x_n) &= \tanh\left(v_1 x_n + b_1\right) \\ h_2(x_n) &= \tanh\left(v_2 x_n + b_2\right) \end{aligned}$$

Solution: Gradient of neural network

$$\frac{\partial E}{\partial c} = -2 \sum_{n=1}^{N} \left(y_n - \hat{y}_n \right)$$

Solution: Gradient of neural network

$$\frac{\partial E}{\partial c} = -2 \sum_{n=1}^{N} \Big(y_n - \hat{y}_n \Big)$$

$$\frac{\partial E}{\partial w_1} = -2 \sum_{n=1}^{N} \Big(\big(y_n - \hat{y}_n \big) h_1(x_n) \Big)$$

Solution: Gradient of neural network

$$\frac{\partial E}{\partial c} = -2 \sum_{n=1}^{N} \left(y_n - \hat{y}_n \right)$$

$$\frac{\partial E}{\partial w_1} = -2 \sum_{n=1}^{N} \left(\left(y_n - \hat{y}_n \right) h_1 \left(x_n \right) \right)$$

$$\frac{\partial E}{\partial b_1} = -2 \sum_{n=1}^{N} \left(\left(y_n - \hat{y}_n \right) w_1 \left(1 - h_1^2(x_n) \right) \right)$$

Solution: Gradient of neural network

$$\frac{\partial E}{\partial c} = -2 \sum_{n=1}^{N} \left(y_n - \hat{y}_n \right)$$

$$\frac{\partial E}{\partial w_1} = -2 \sum_{n=1}^{N} \left(\left(y_n - \hat{y}_n \right) h_1 \left(x_n \right) \right)$$

$$\frac{\partial E}{\partial b_1} = -2 \sum_{n=1}^{N} \left(\left(y_n - \hat{y}_n \right) w_1 \left(1 - h_1^2 (x_n) \right) \right)$$

$$\frac{\partial E}{\partial v_1} = -2 \sum_{n=1}^{N} \left(\left(y_n - \hat{y}_n \right) w_1 \left(1 - h_1^2 (x_n) \right) \right) x_n$$

Analysis of gradient

- Gradient scales with the error $y_n - \hat{y}_n$
- If $h_1(x_n)$ saturates at -1 or +1, the term $1 - h_1^2(n)$ is zero

Partial derivatives

$$\frac{\partial E}{\partial c} = -2 \sum_{n=1}^{N} \Big(y_n - \hat{y}_n \Big)$$

$$\frac{\partial E}{\partial w_1} = -2 \sum_{n=1}^{N} \Big((y_n - \hat{y}_n) h_1(x_n) \Big)$$

$$\frac{\partial E}{\partial b_1} = -2 \sum_{n=1}^{N} \Big((y_n - \hat{y}_n) w_1 (1 - h_1^2(n)) \Big)$$

$$\frac{\partial E}{\partial v_1} = -2 \sum_{n=1}^{N} \Big((y_n - \hat{y}_n) w_1 (1 - h_1^2(n)) \Big) x_n$$

Tasks

Tasks

Tasks today

1. Work through the notebook `08-GradientDescentLinearRegression.ipynb`
2. Work through the notebook `08-GradientDescentNeuralNet.ipynb`
3. Today's feedback group
   - Nicholas Borch
   - Alfred Fonnesbech Aqraou
   - Josefine Høgsted Voglhofer
   - Rasmus Bernth Linnemann

Lab report hand in

- Lab 3: Image segmentation (Deadline: Thursday 26 October 20:00)