Introduction to Optimization

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https://github.com/ichatnun/MRI-simple-optimization-workshop

Optimization

- Goal: Given $f(x) = b$, recover x from b

unknown

input

x

system

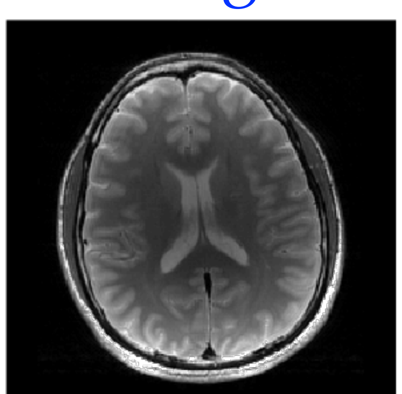
sensor / scanner

f

observation

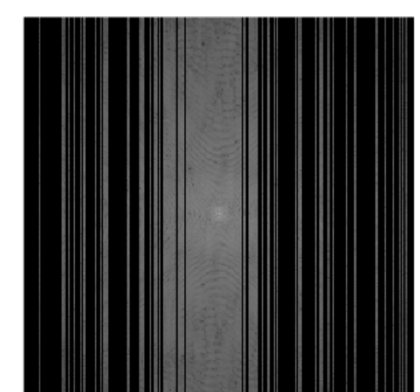
b

Underlying image



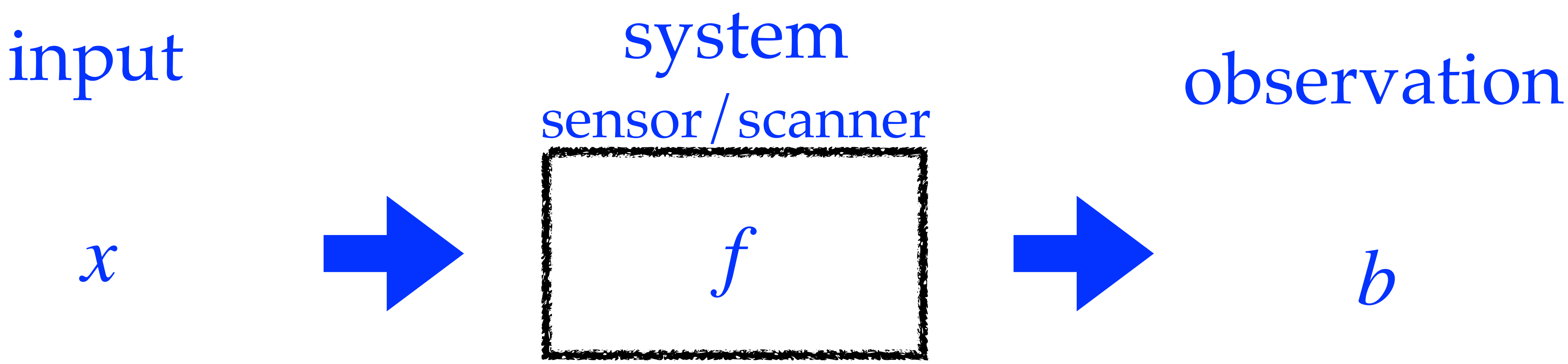
MRI machine

Acquired k-space data



Optimization

- Goal: Given $f(x) = b$, recover x from b



Idea 1: Randomly guess lots of x's and pick the best one

What does it mean to be "the best one"?

For simplicity, we will use the Euclidean distance between $f(x)$ and b. Specifically, we want to minimize the following loss function

$$L(x) = ||f(x) - b||_2^2$$

Optimization

$$L(x) = ||f(x) - b||_2^2$$

$$\begin{bmatrix} 1 \\ 3 \\ 1 \end{bmatrix} \quad \begin{bmatrix} 2 \\ 3 \\ 0 \end{bmatrix}$$

acquired / observed data

Try x_1 $\xrightarrow{\text{apply } f \text{ to it}}$ $f(x_1)$

$$L(x_1) = ||f(x_1) - b||_2^2 = (1-2)^2 + (3-3)^2 + (1-0)^2 = 2$$

Optimization

$$L(x) = ||f(x) - b||_2^2$$

$$\begin{bmatrix}1\\3\\0\end{bmatrix} \quad \begin{bmatrix}2\\3\\0\end{bmatrix}$$

acquired / observed data

Try x_2 $\xrightarrow{\text{apply } f \text{ to it}}$ $f(x_2)$

$$L(x_1) = ||f(x_1) - b||_2^2 = (1-2)^2 + (3-3)^2 + (1-0)^2 = 2$$

$$L(x_2) = ||f(x_2) - b||_2^2 = (1-2)^2 + (3-3)^2 + (0-0)^2 = 1$$

Better guess

Example 1: Random guess

input　　system　　observation

$$x \rightarrow \boxed{f} \rightarrow b$$

$$f(x) = b$$

Given

- The observation b
- The applyF() function, which computes $f(x)$ whenever an x is given $\quad applyF(x) \rightarrow f(x)$
- The loss() function, which computes the difference between the given two vectors $\quad loss(b_1, b_2) \rightarrow ||b_1 - b_2||_2^2$

Goal: Try to recover x using the code provided in ex1.m

Hint: Each entry of the true x has the value between 0 and 1

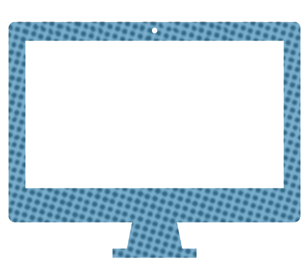
Optimization

- Goal: Given $f(x) = b$, recover x from b

input　　system　　observation

$$x \rightarrow \boxed{\; f \;} \rightarrow b$$

Idea 2: Write a MATLAB program to generate lots of x's in a grid search manner and automatically pick the best one



$$\rightarrow \quad \begin{matrix} \begin{bmatrix}0\\0\\0\end{bmatrix} & \begin{bmatrix}0.1\\0\\0\end{bmatrix} & \begin{bmatrix}0.2\\0\\0\end{bmatrix} & \cdots & \begin{bmatrix}0.9\\0\\0\end{bmatrix} & \begin{bmatrix}1\\0\\0\end{bmatrix} \\ \vdots & & & & & \vdots \\ \begin{bmatrix}1\\1\\0\end{bmatrix} & \begin{bmatrix}1\\1\\0.1\end{bmatrix} & \begin{bmatrix}1\\1\\0.2\end{bmatrix} & \cdots & \begin{bmatrix}1\\1\\0.9\end{bmatrix} & \begin{bmatrix}1\\1\\1\end{bmatrix} \end{matrix}$$

Example 2: Grid Search

input | system | observation

x $\rightarrow$ $\boxed{f}$ $\rightarrow$ b

$$f(x) = b$$

Given

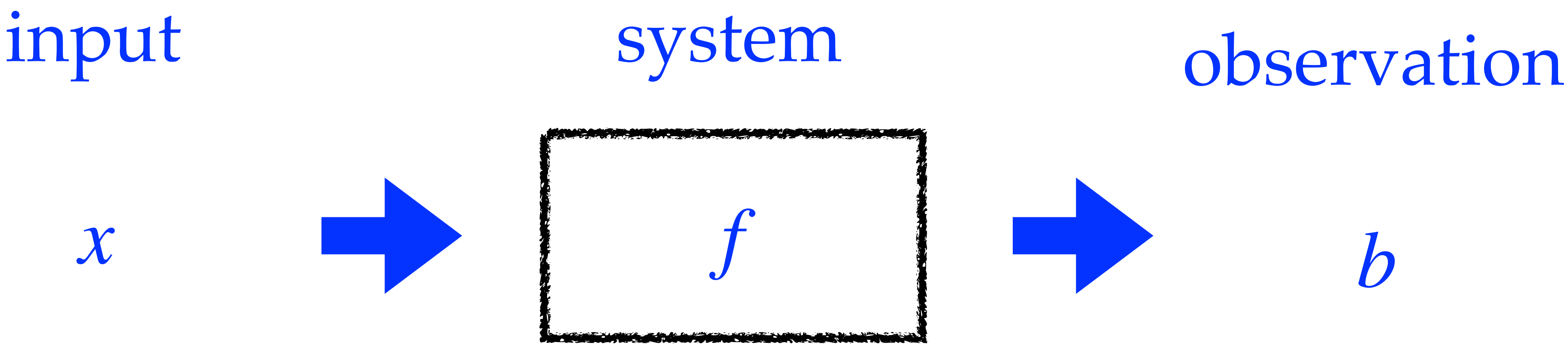
- The observation b
- The applyF() function, which computes $f(x)$ whenever an x is given $\quad applyF(x) \rightarrow f(x)$
- The loss() function, which computes the difference between the given two vectors $\quad loss(b_1, b_2) \rightarrow ||b_1 - b_2||_2^2$

Goal: Try to recover x using the code provided in ex2.m

Hint: Each entry of the true x has the value between 0 and 1

Optimization

- Goal: Given $f(x) = b$, recover x from b



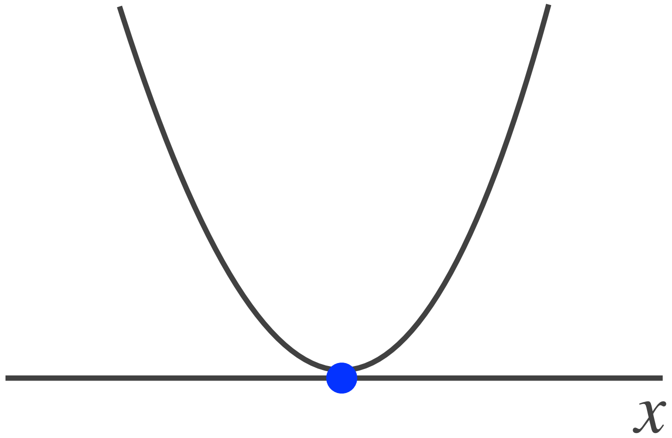
Guessing the solution is not very efficient…

Idea 3: Gradient descent

Gradient Descent

- Goal: Find x that minimizes the following loss function

$$L(x) = x^2$$



Method 1: Compute the derivative and set it to 0

Gradient $\dfrac{dL(x)}{dx} = \dfrac{dx^2}{dx} = 2x$ $= 0$ $x = 0$

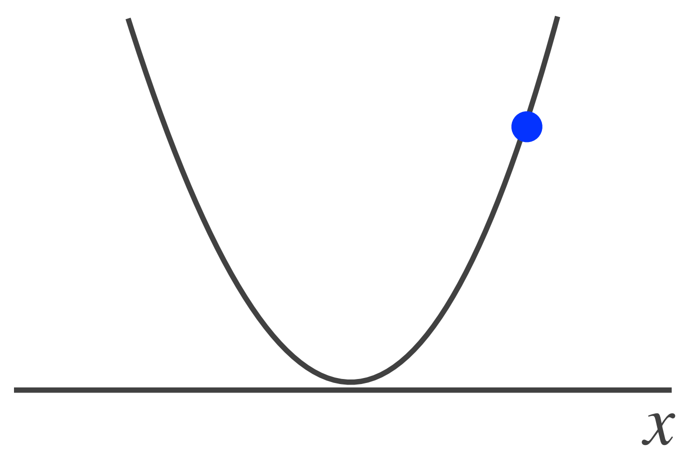
In many cases, it is not simple to compute the gradient with respect to x.

Even when we have a way to compute the gradient and manage to set it to zero, we might not be able to get a closed-form solution for it.

Gradient Descent

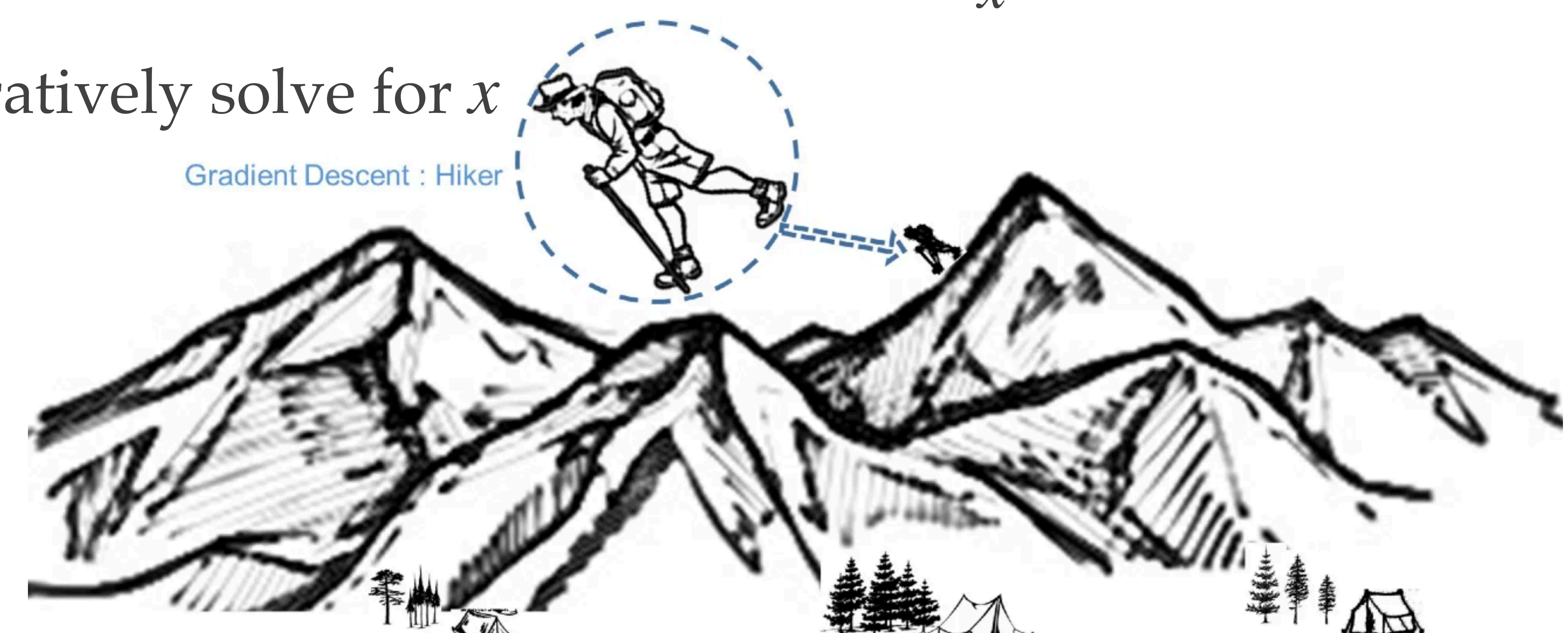
- Goal: Find x that minimizes the following loss function

$$L(x) = x^2$$



- Randomly start somewhere
- Gradually move to the minimum of the function

Method 2: Iteratively solve for x

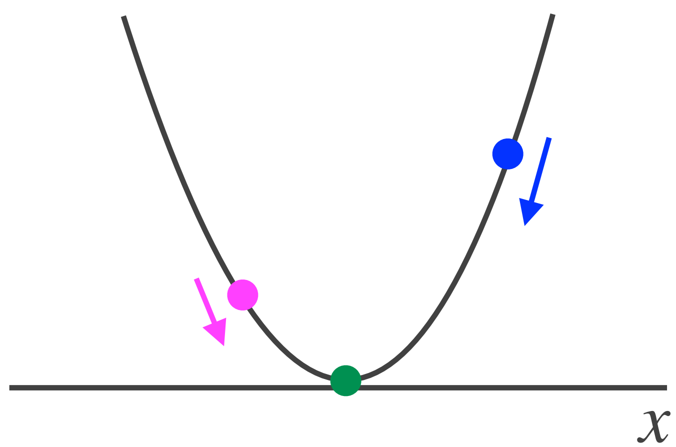


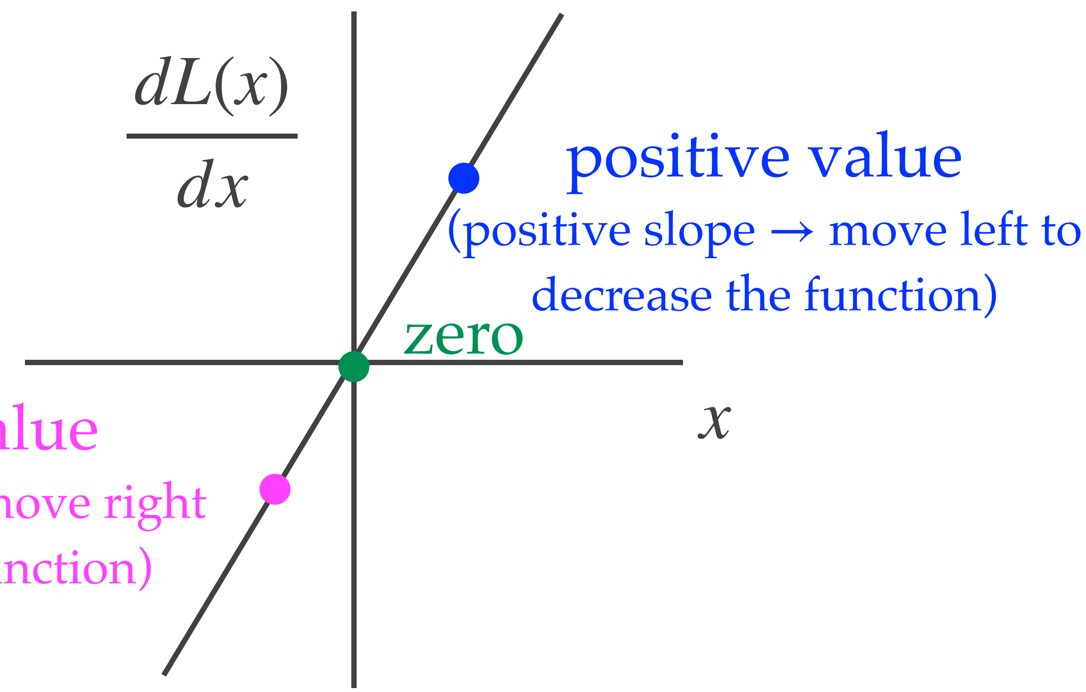
Gradient Descent for Logistic Regression Simplified – Step by Step Visual Guide

Gradient Descent

- Goal: Find x that minimizes the following loss function

$$L(x) = x^2$$





Method 2: Iteratively solve for x

1. Guess an initial solution x_0 and pick α

For $k = 0,1,2,\ldots$

Iteration k

2. Compute $\frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = 2x\,\Big|_{x=x_{(k)}} = 2x_{(k)}$

3. Compute a new solution $x_{(k+1)} := x_{(k)} - \alpha\frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = x_{(k)} - \alpha * 2x_{(k)}$

step size/learning rate α indicates how far we want to move

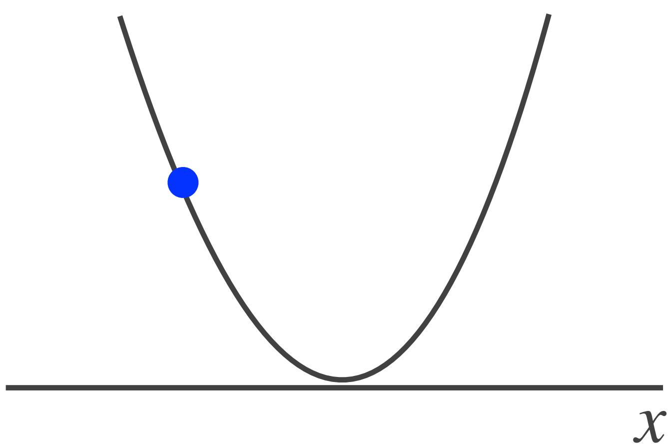
4. Repeat step 2 and 3 until converge

The negative of the gradient $-\frac{dL(x)}{dx}$ tells us the direction we should move to decrease the function

Gradient Descent

- Goal: Find w that minimizes the following loss function

$$L(x) = x^2$$



$$x_{(0)} = -2, \alpha = 0.5$$

$$x_{(1)} = x_{(0)} - \alpha * 2x_{(0)} = -2 - 0.5 * 2 * -2 = 0$$

$$x_{(2)} = x_{(1)} - \alpha * 2x_{(1)} = 0$$

$$x_{(3)} = x_{(2)} - \alpha * 2x_{(2)} = 0$$

Method 2: Iteratively solve for x

1. Guess an initial solution x_0 and pick α

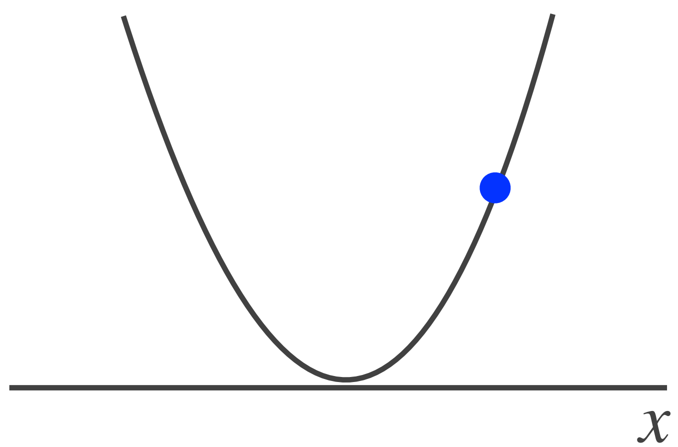
For $k = 0,1,2,\ldots$

2. Compute $\frac{dL(x)}{dx}|_{x=x_{(k)}} = 2x|_{x=x_{(k)}} = 2x_{(k)}$
3. Compute a new solution $x_{(k+1)} := x_{(k)} - \alpha \frac{dL(x)}{dx}|_{x=x_{(k)}} = x_{(k)} - \alpha * 2x_{(k)}$
4. Repeat step 2 and 3 until converge

Gradient Descent

- Goal: Find w that minimizes the following loss function

$$L(x) = x^2$$



$$x_{(0)} = 2, \alpha = 0.5$$

$$x_{(1)} = x_{(0)} - \alpha * 2x_{(0)} = 2 - 0.5 * 2 * 2 = 0$$

$$x_{(2)} = x_{(1)} - \alpha * 2x_{(1)} = 0$$

$$x_{(3)} = x_{(2)} - \alpha * 2x_{(2)} = 0$$

Method 2: Iteratively solve for x

1. Guess an initial solution x_0 and pick α

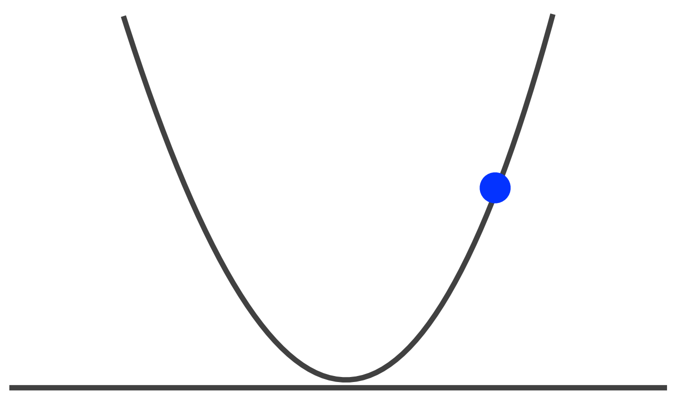
For $k = 0,1,2,...$

2. Compute $\frac{dL(x)}{dx}\big|_{x=x_{(k)}} = 2x\big|_{x=x_{(k)}} = 2x_{(k)}$
3. Compute a new solution $x_{(k+1)} := x_{(k)} - \alpha \frac{dL(x)}{dx}\big|_{x=x_{(k)}} = x_{(k)} - \alpha * 2x_{(k)}$
4. Repeat step 2 and 3 until converge

Gradient Descent

- Goal: Find w that minimizes the following loss function

$$L(x) = x^2$$



$$x_{(0)} = 2, \alpha = 0.25$$

$$x_{(1)} = x_{(0)} - \alpha * 2x_{(0)} = 2 - 0.25 * 2 * 2 = 1$$

$$x_{(2)} = x_{(1)} - \alpha * 2x_{(1)} = 1 - 0.25 * 2 * 1 = 0.5$$

$$x_{(3)} = x_{(2)} - \alpha * 2x_{(2)} = 0.5 - 0.25 * 2 * 0.5 = 0.25$$

$$x_{(4)} = x_{(3)} - \alpha * 2x_{(3)} = 0.125$$

$$x_{(5)} = x_{(4)} - \alpha * 2x_{(4)} = 0.0625$$

Method 2: Iteratively solve for x

1. Guess an initial solution x_0 and pick α

For $k = 0,1,2,...$

2. Compute $\frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = 2x\big|_{x=x_{(k)}} = 2x_{(k)}$

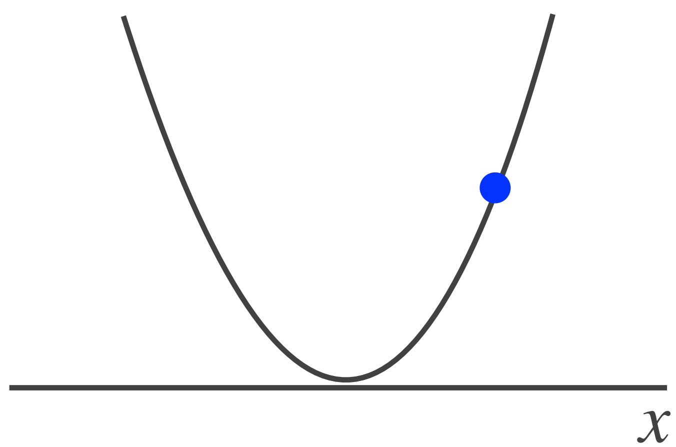
3. Compute a new solution $x_{(k+1)} := x_{(k)} - \alpha \frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = x_{(k)} - \alpha * 2x_{(k)}$

4. Repeat step 2 and 3 until converge

Gradient Descent

- Goal: Find w that minimizes the following loss function

$$L(x) = x^2$$



$$x_{(0)} = 2, \alpha = 1$$

$$x_{(1)} = x_{(0)} - \alpha * 2x_{(0)} = 2 - 1 * 2 * 2 = -2$$

$$x_{(2)} = x_{(1)} - \alpha * 2x_{(1)} = -2 - 1 * 2 * -2 = 2$$

$$x_{(3)} = x_{(2)} - \alpha * 2x_{(2)} = -2$$

$$x_{(4)} = x_{(3)} - \alpha * 2x_{(3)} = 2$$

$$x_{(5)} = x_{(4)} - \alpha * 2x_{(4)} = -2$$

Method 2: Iteratively solve for x

1. Guess an initial solution x_0 and pick α

For $k = 0,1,2,...$

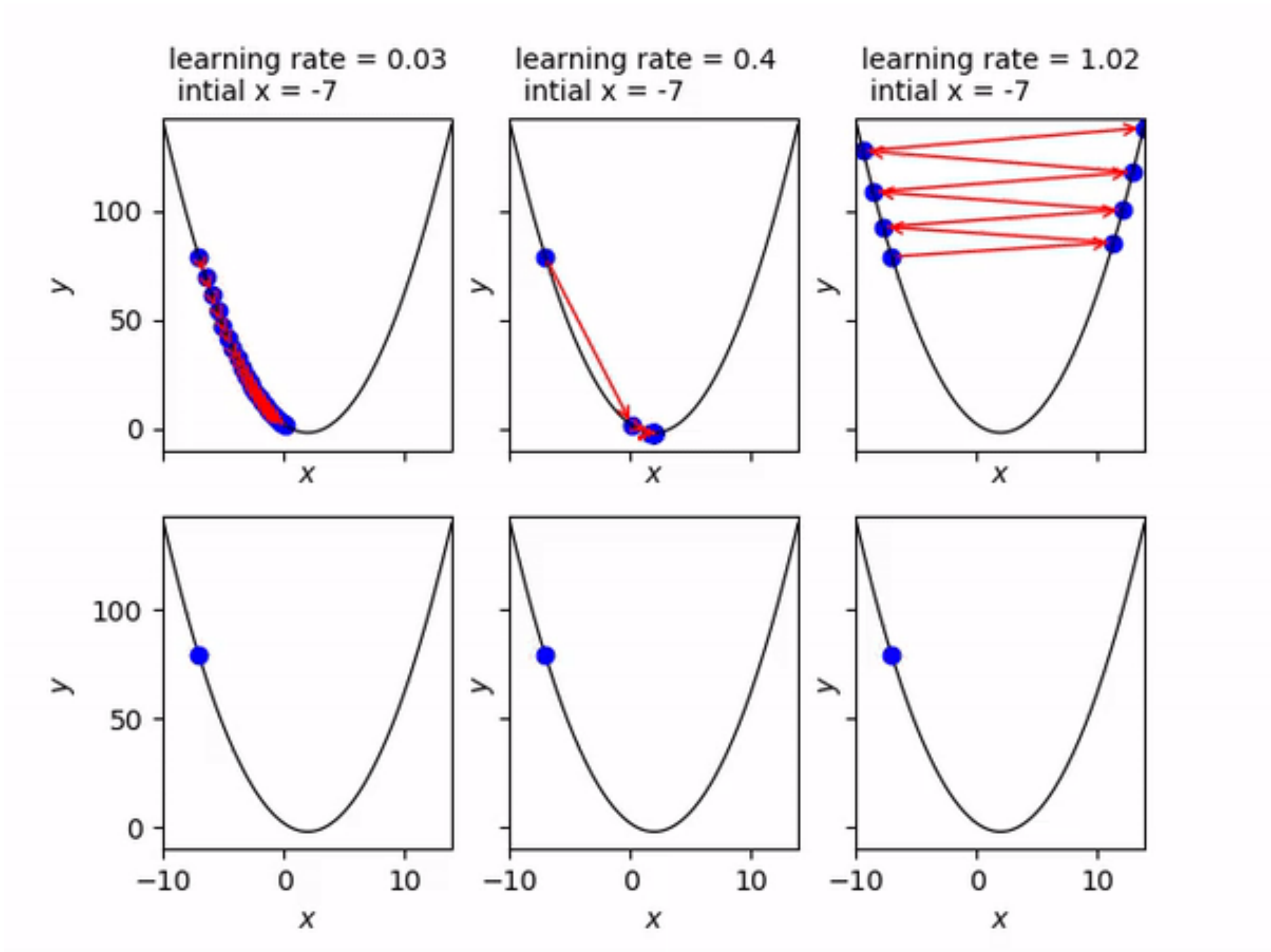
2. Compute $\frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = 2x\,\Big|_{x=x_{(k)}} = 2x_{(k)}$

3. Compute a new solution $x_{(k+1)} := x_{(k)} - \alpha \frac{dL(x)}{dx}\Big|_{x=x_{(k)}} = x_{(k)} - \alpha * 2x_{(k)}$

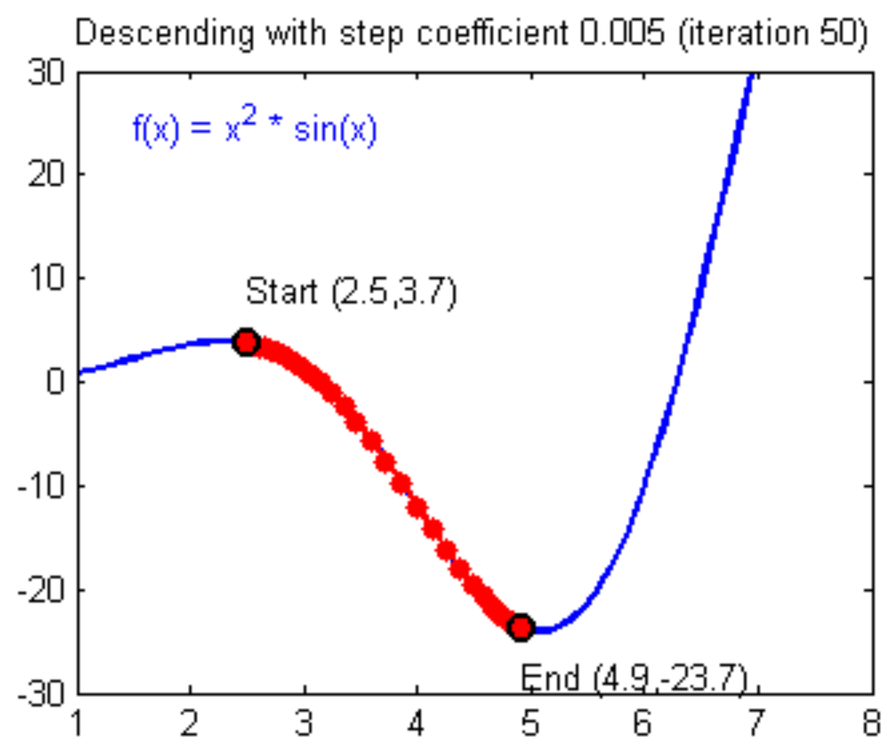
4. Repeat step 2 and 3 until converge

α: learning rate

Gradient Descent: Learning Rate



Fixed learning rate



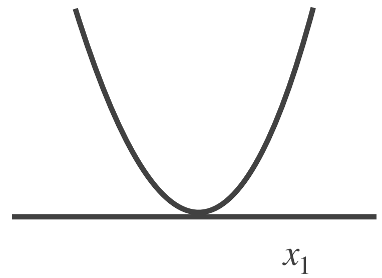
Adaptive learning rate

Deep Learning, NeuroEvolution & Extreme Learning Machines

Gradient

1-dimensional case

$$L(x_1) = x_1^2$$



Derivative of $L(x_1)$

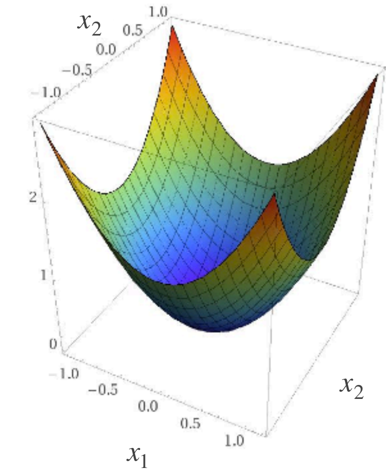
$$\frac{dL(x_1)}{dx_1} = \frac{dx_1^2}{dx_1} = 2x_1$$

Weight update

$$x_{1,(k+1)} := x_{1,(k)} - \alpha \frac{dL(x_1)}{dx_1}\Big|_{x_1 = x_{1,(k)}}$$

$$= x_{1,(k)} - 2x_{1,(k)}$$

2-dimensional case



$$L(x_1, x_2) = x_1^2 + x_2^2$$

Partial derivatives of $L(x_1, x_2)$

$$\frac{\partial L(x_1, x_2)}{\partial x_1} = \frac{\partial}{\partial x_1}(x_1^2 + x_2^2) = 2x_1$$

$$\frac{\partial L(x_1, x_2)}{\partial x_2} = \frac{\partial}{\partial x_2}(x_1^2 + x_2^2) = 2x_2$$

Gradient $\nabla_x L(x_1, x_2)$

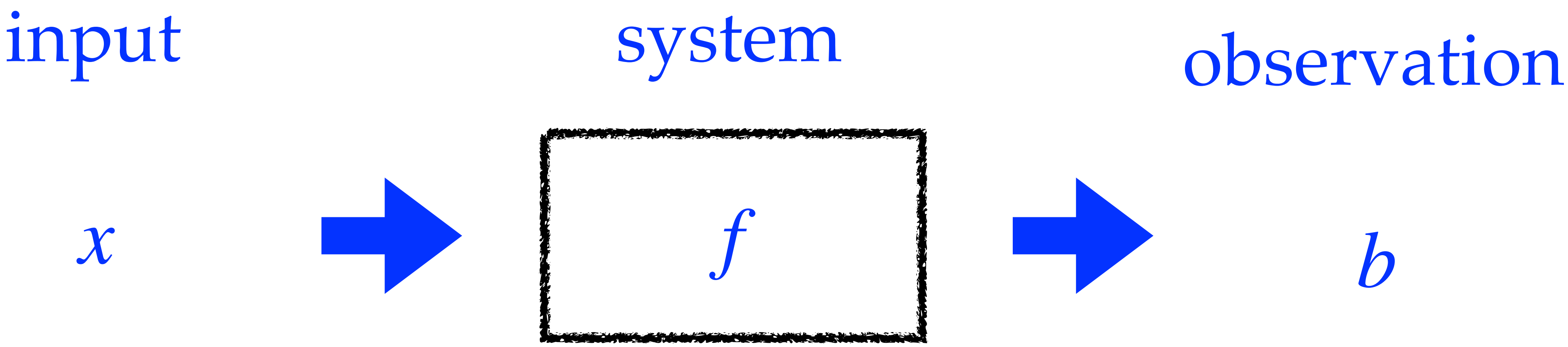
Weight update

$$\begin{bmatrix} x_{1,(k+1)} \\ x_{2,(k+1)} \end{bmatrix} = \begin{bmatrix} x_{1,(k)} \\ x_{2,(k)} \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial L(x_1, x_2)}{\partial x_1}\Big|_{x_1 = x_{1,(k)}} \\ \frac{\partial L(x_1, x_2)}{\partial x_2}\Big|_{x_2 = x_{2,(k)}} \end{bmatrix}$$

$$= \begin{bmatrix} x_{1,(k)} \\ x_{2,(k)} \end{bmatrix} - \alpha \begin{bmatrix} 2x_{1,(k)} \\ 2x_{2,(k)} \end{bmatrix}$$

Optimization

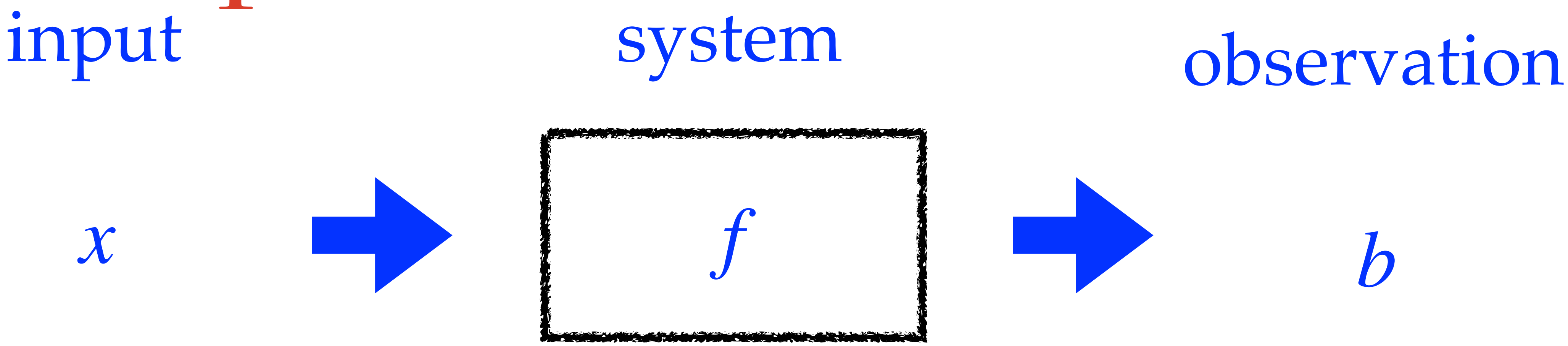
- Goal: Given $f(x) = b$, recover x from b



Guessing the solution is not very efficient…

Idea 3: Gradient descent

Example 3: Gradient Descent



$$f(x) = b$$

Given

- The observation b
- The applyF() function, which computes $f(x)$ whenever an x is given
- The loss() function, which computes the difference between the given two vectors
- The computeGradient() function, which computes the gradient of the loss function: $L(x) = ||f(x) - b||_2^2$

Goal: Try to recover x using the code provided in ex3.m

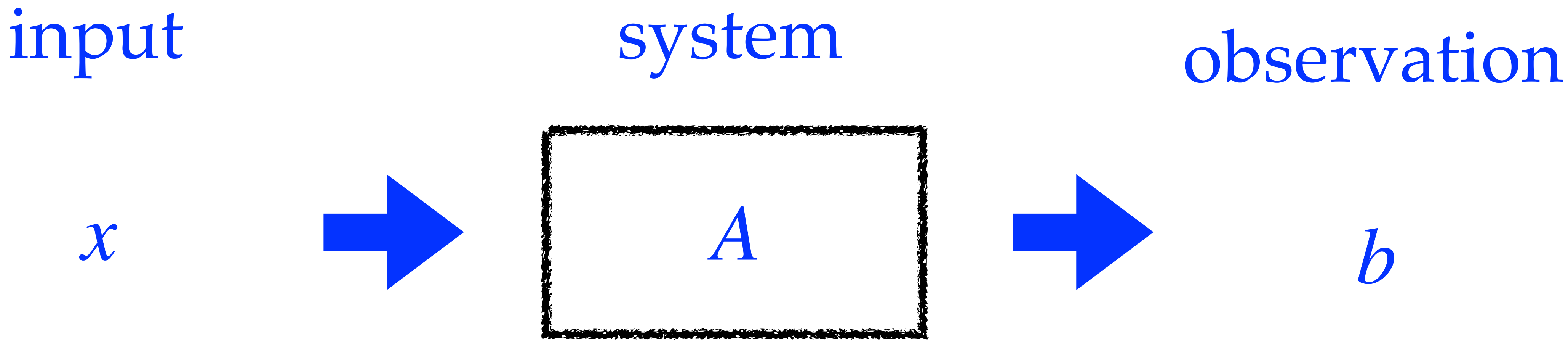
Hints

- If we take a look at the code, we will see that $f(x) = Ax$
- The gradient of the loss function has a nice form: $\nabla_x L(x) = \nabla_x ||f(x) - b||_2^2 = \nabla_x ||Ax - b||_2^2 = 2A^*(Ax - b)$
- The update equation becomes

$$x_{(k+1)} := x_{(k)} - \alpha \times 2A^*(Ax_{(k)} - b)$$

Linear System

- Goal: Given $Ax = b$, recover x from b



$$1.3 = x_1 + 0 \cdot x_2 + 4x_3$$
$$1.5 = 0.2x_1 + 3x_2 + x_3$$
$$0.4 = 0 \cdot x_1 + x_2 + 0 \cdot x_3$$

$$\begin{bmatrix} 1.3 \\ 1.5 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 4 \\ 0.2 & 3 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\min_x \|Ax - b\|_2^2$$

Unique solution

$$x = A^{-1}b = \begin{bmatrix} 0.5 \\ 0.4 \\ 0.2 \end{bmatrix}$$

Underdetermined system

$$1.3 = x_1 + 0 \cdot x_2 + 4x_3$$
$$1.5 = 0.2x_1 + 3x_2 + x_3$$
$$0.4 = 0 \cdot x_1 + x_2 + 0 \cdot x_3$$

$$[1.3] = [1 \quad 0 \quad 4] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\min_x \|Ax - b\|_2^2$$

Possible solutions

$$\begin{bmatrix} 0.5 \\ 0.4 \\ 0.2 \end{bmatrix}, \begin{bmatrix} 0.0765 \\ 0.0 \\ 0.3509 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0.325 \end{bmatrix}, \ldots$$

Example 4: Confirm that the results shown here are accurate using ex4.m

$$1.3 = x_1 + 0 \cdot x_2 + 4x_3$$
$$1.5 = 0.2x_1 + 3x_2 + x_3$$
$$0.4 = 0 \cdot x_1 + x_2 + 0 \cdot x_3$$

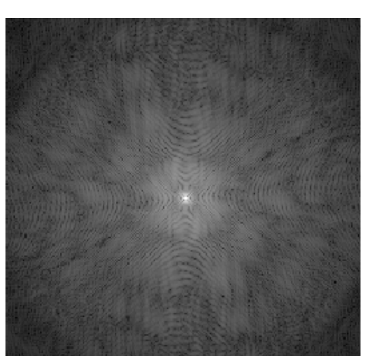
$$\begin{bmatrix} 1.3 \\ 1.5 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 4 \\ 0.2 & 3 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\min_x \|Ax - b\|_2^2$$

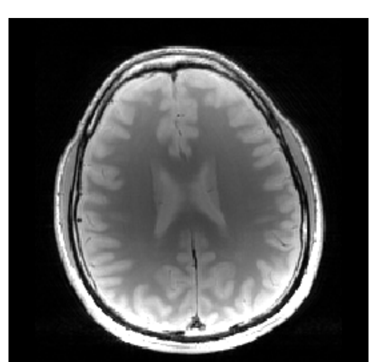
Unique solution

$$x = A^{-1}b = \begin{bmatrix} 0.5 \\ 0.4 \\ 0.2 \end{bmatrix}$$

Fully-sampled



Unique solution



Underdetermined system

$$1.3 = x_1 + 0 \cdot x_2 + 4x_3$$
$$1.5 = 0.2x_1 + 3x_2 + x_3$$
$$0.4 = 0 \cdot x_1 + x_2 + 0 \cdot x_3$$

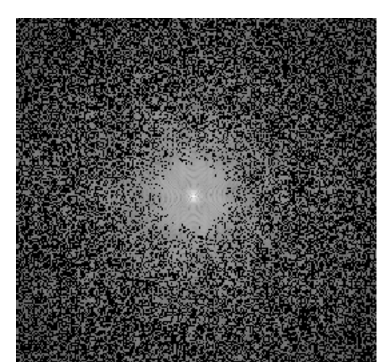
$$\begin{bmatrix} 1.3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\min_x \|Ax - b\|_2^2$$

Possible solutions

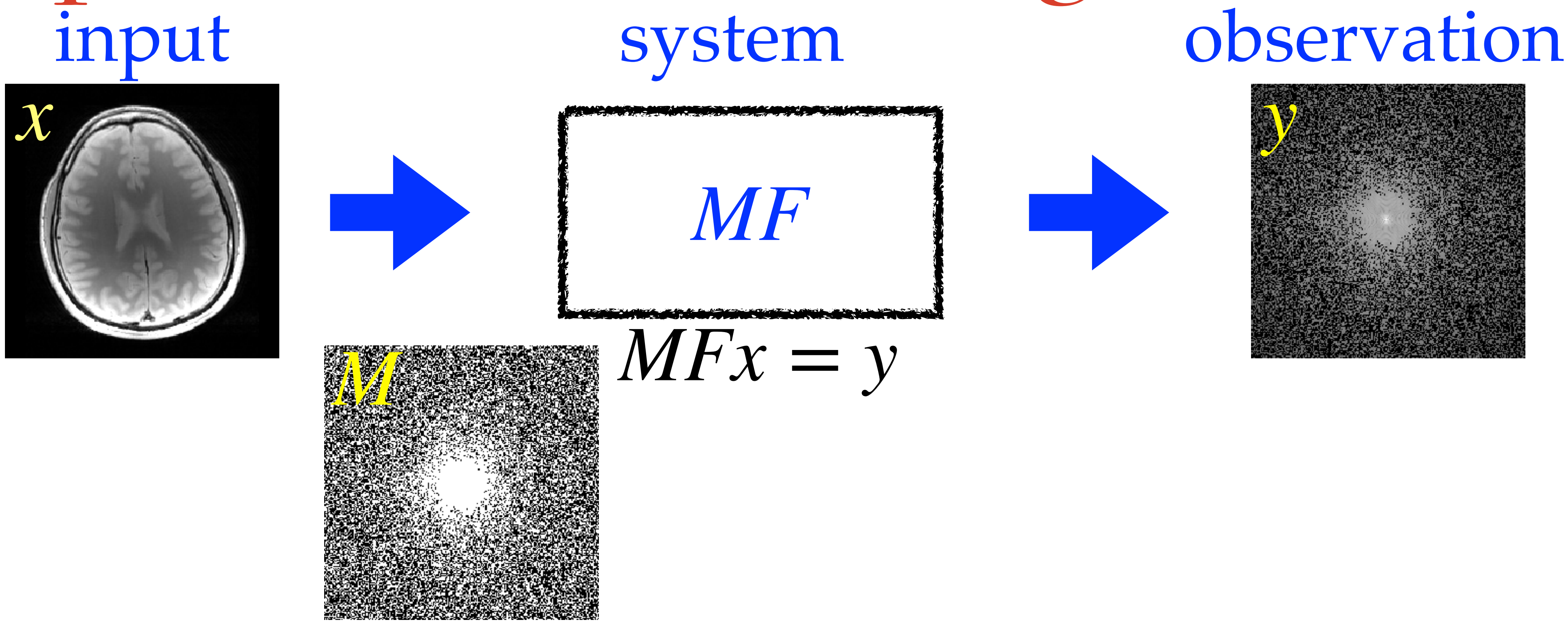
$$\begin{bmatrix} 0.5 \\ 0.4 \\ 0.2 \end{bmatrix}, \begin{bmatrix} 0.0765 \\ 0.0 \\ 0.3509 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0.325 \end{bmatrix}, \ldots$$

Undersampled



one possible solution

Example 5: Tikhonov Regularization

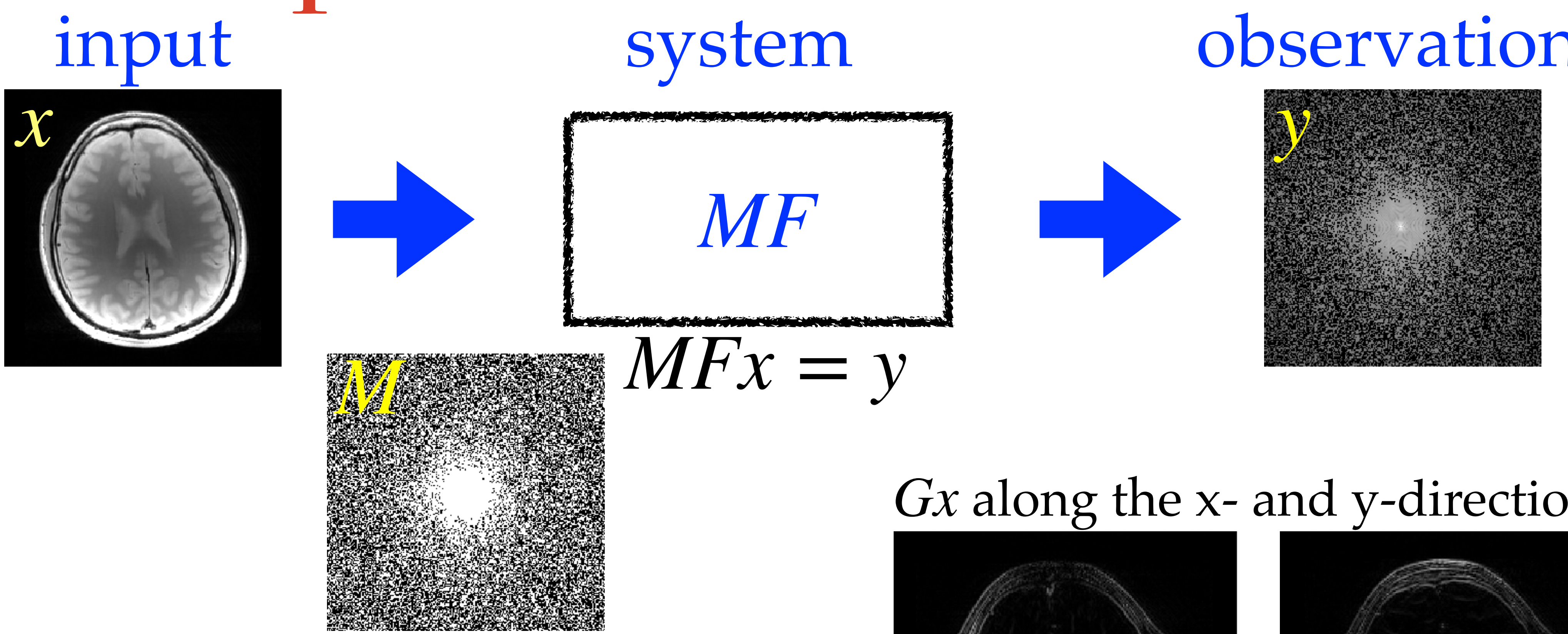


- Approach: Solve $\min_x L(x) = \min_x \|MFx\ -\ y\|_2^2 + \lambda\|x\|_2^2$ using gradient descent (ex4.m), enforcing the L2-norm on the image
- The update equation:

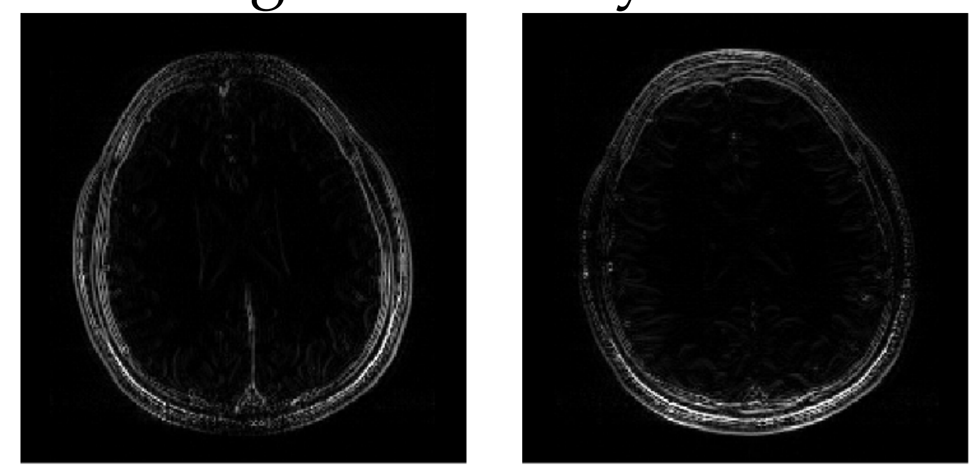
$$x_{(k+1)} := x_{(k)} - \alpha \times \underbrace{[2F^*M^*(MFx_{(k)} - y) + 2\lambda x_{(k)}]}_{\text{gradient of } L(x)}$$

- Notes
  - Try adjusting the parameters in ex5.m such as
    - The regularization parameter λ
      - $\lambda = 0 \rightarrow$ No regularization (under-determined system of equations)
    - The learning rate α
    - The reduction factor R

Example 6: Total Variation



Gx along the x- and y-directions



- Approach: Solve $\min_{x} L(x) = \min_{x} \|MFx - y\|_2^2 + \lambda \|Gx\|_1$ using (sub)gradient descent (ex6.m), enforcing sparsity on the image in the finite difference domain (Gx)
- The update equation:

$$x_{(k+1)} := x_{(k)} - \alpha \times [2F^*M^*(MFx_{(k)} - y) + 2G^*sign(Gx_{(k)})]$$