Machine Learning in Imaging

BME 590L
Roarke Horstmeyer

Lecture 5: Ingredients for Machine Learning

Outline

- Review spectral unmixing (last class)
- From optimization to machine learning
- Ingredients for ML
- Example: linear classification of images
  - Train/test data
  - Linear regression model
  - 3 ways to solve

Last time: simple example of spectral unmixing

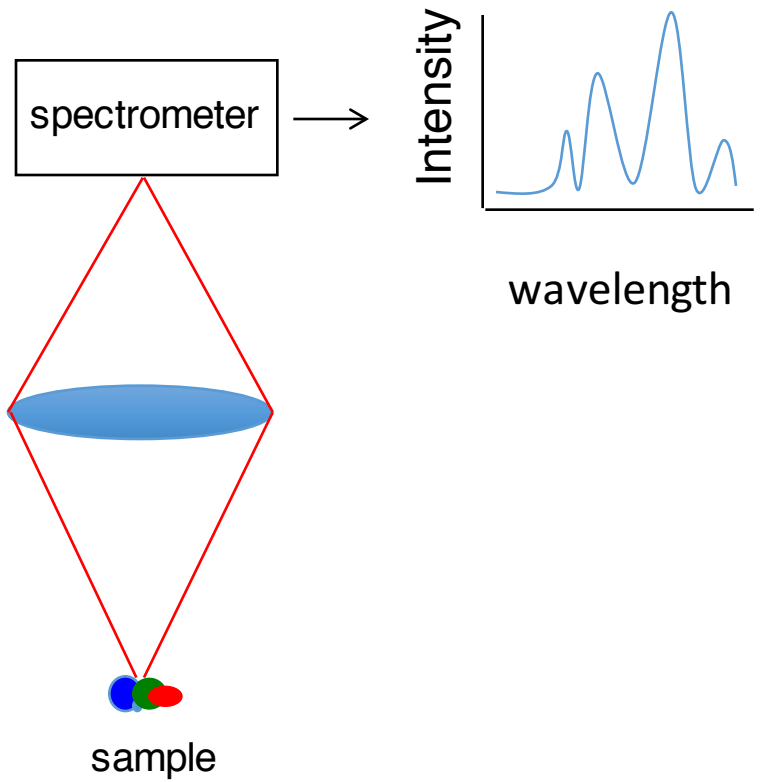
(For whatever reason, whenever I get confused about optimization, I think about this example)

The setup:

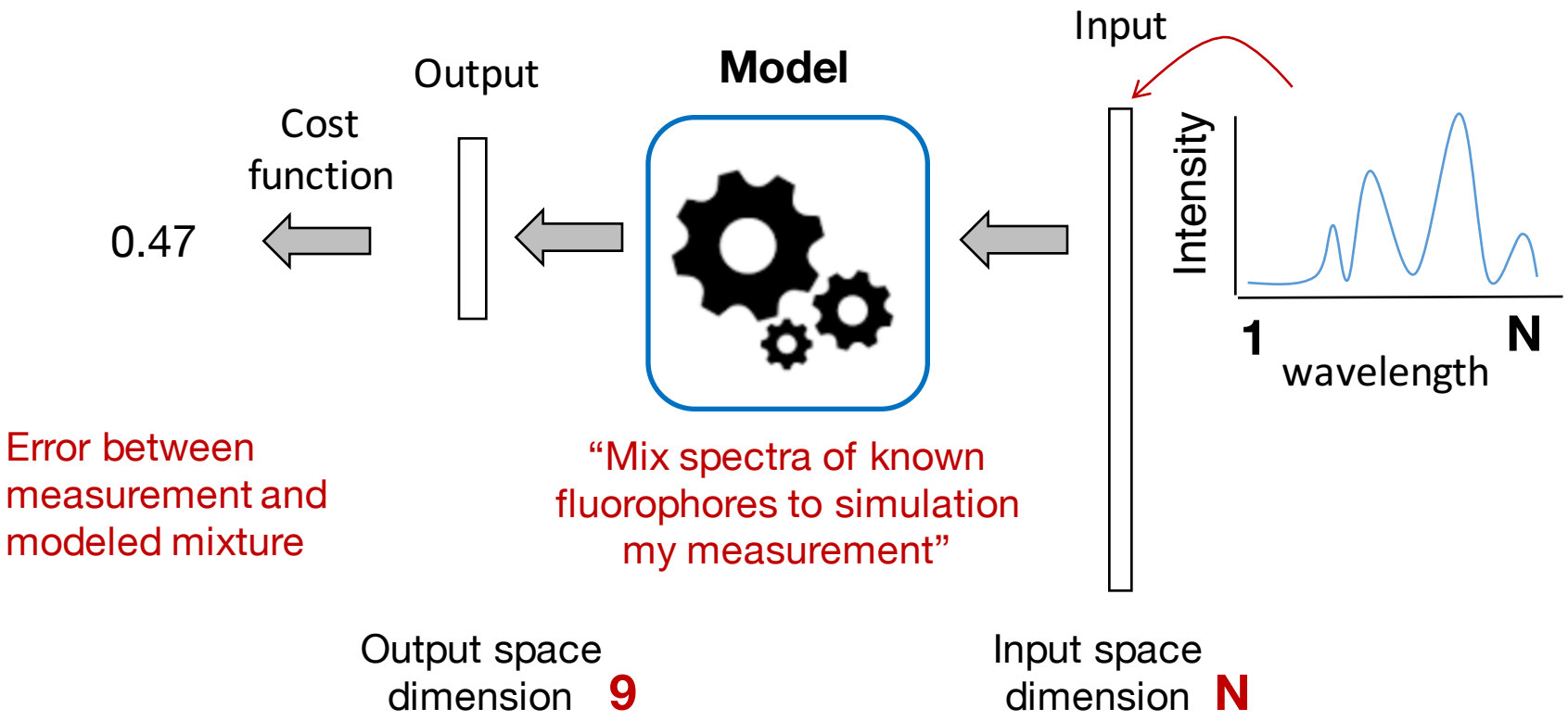
- measure the color (spectral) response of a sample (e.g., how much red, green and blue there is, or several hundred measurements of its different colors).

- You know that the sample can only contain 9 different fluorophores.

- What % of each fluorophores is in your sample?



Optimization pipeline for spectral unmixing



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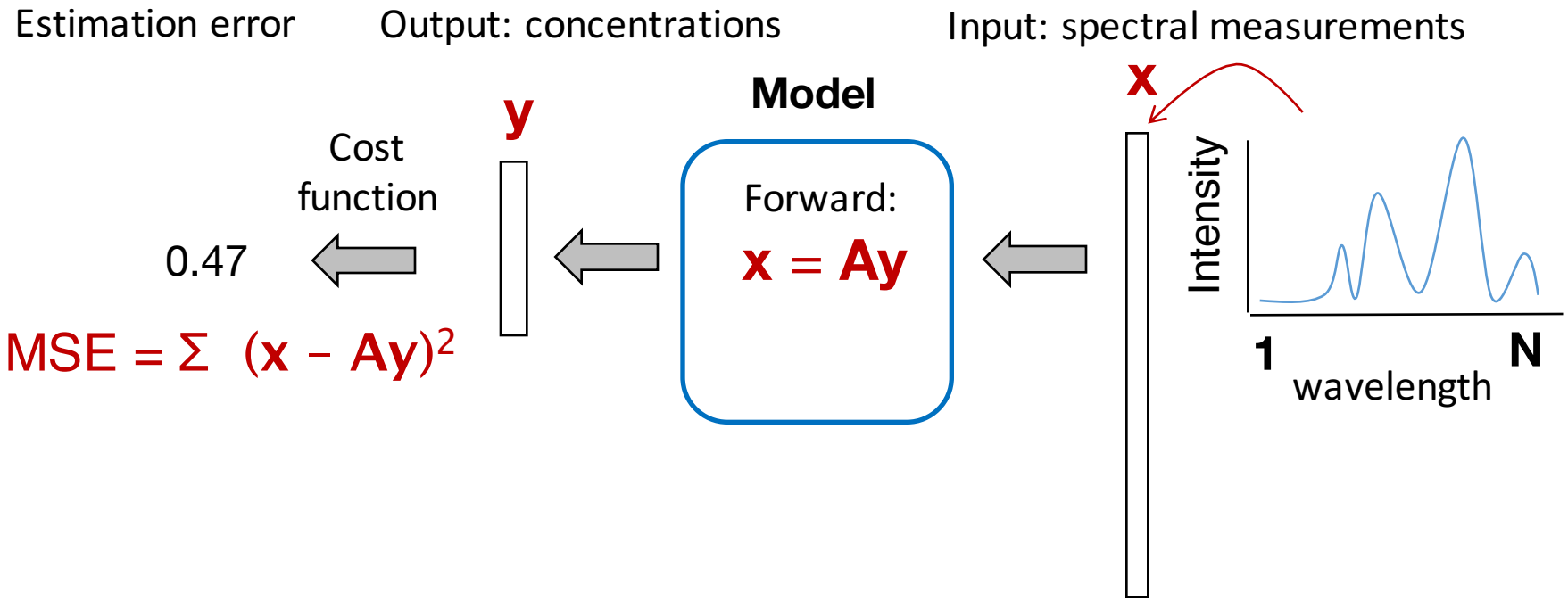
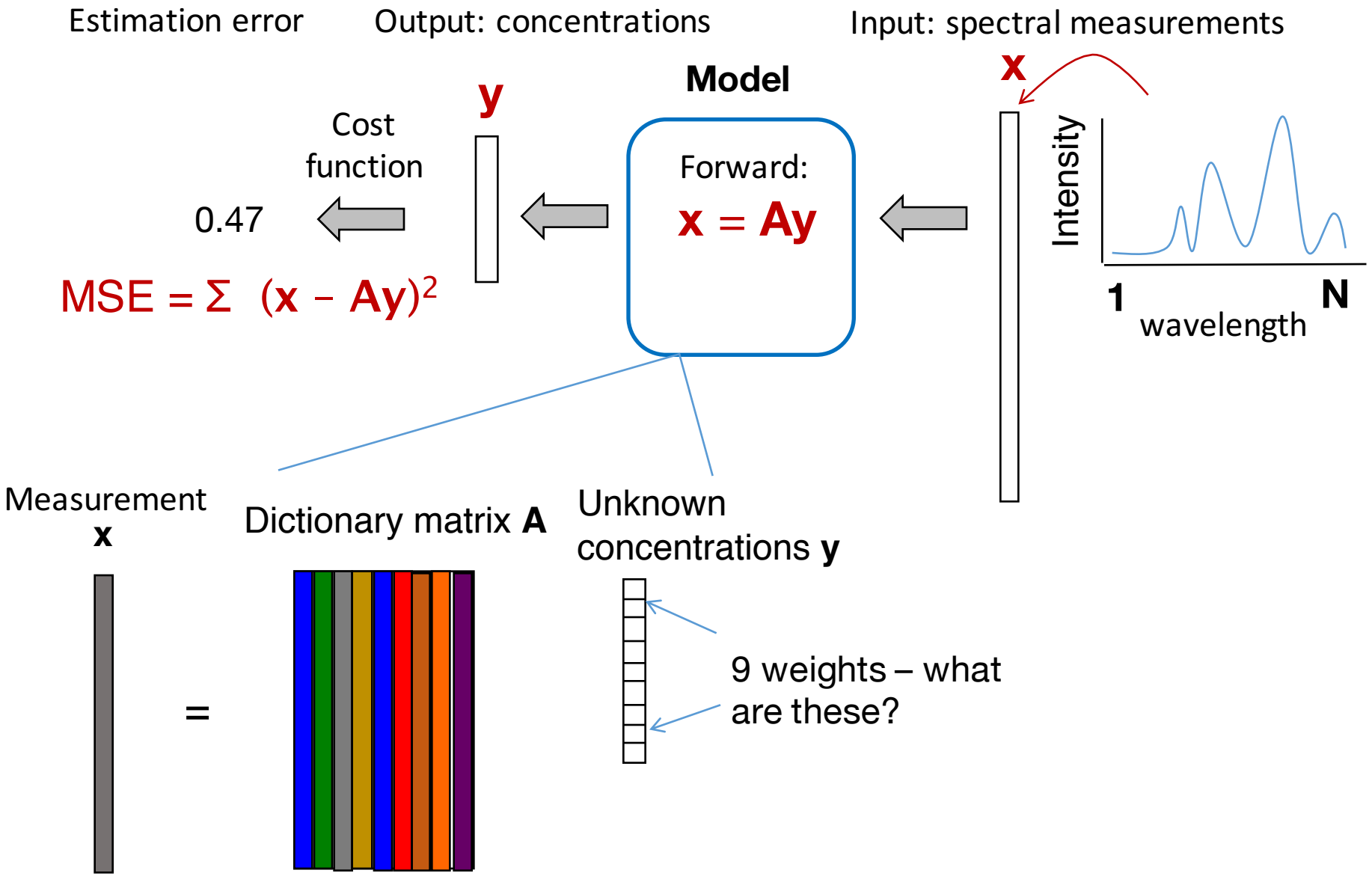


*Note: notation changed from last time to be consistent with we'll use in the future

Optimization pipeline for spectral unmixing



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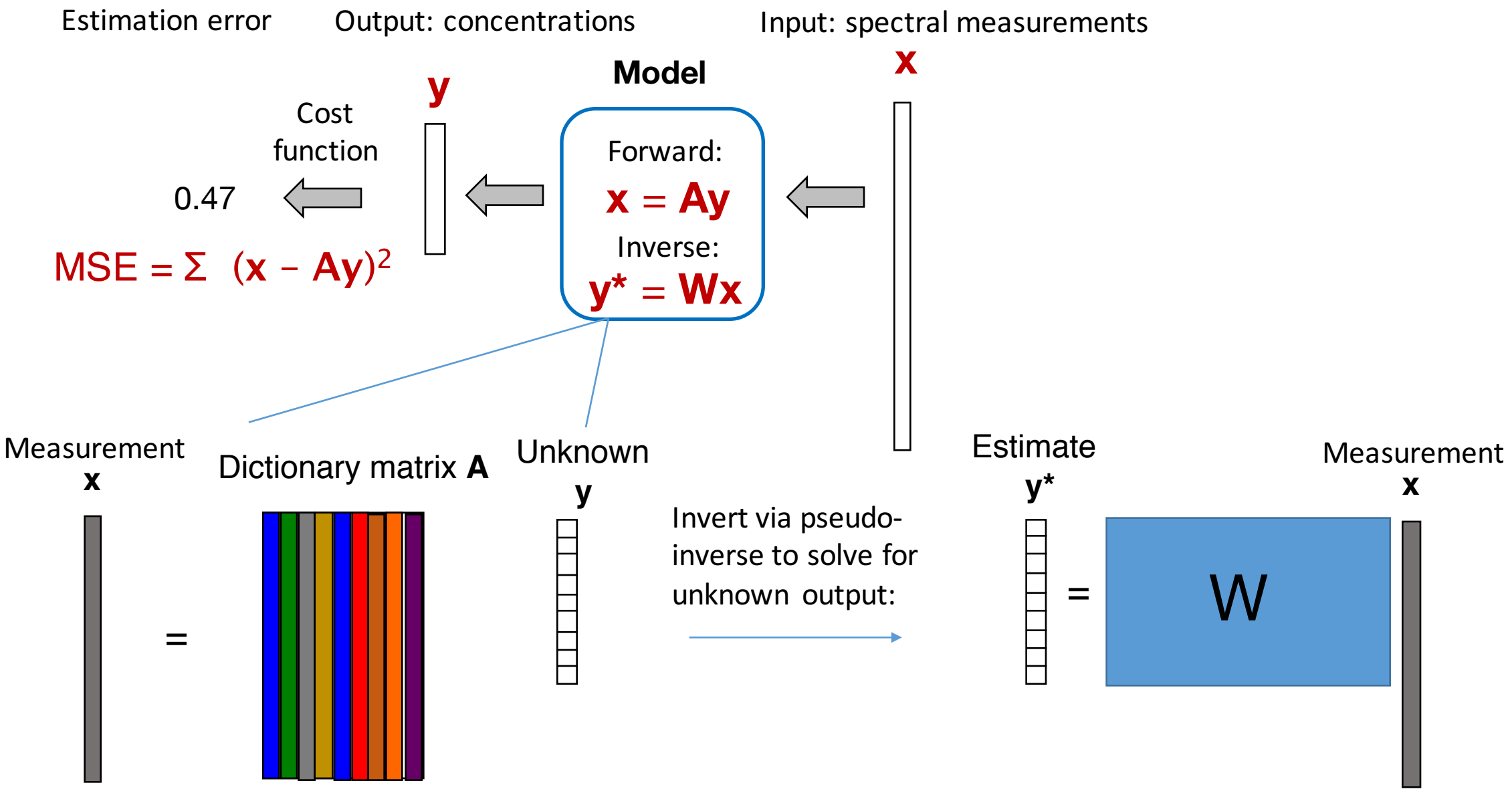

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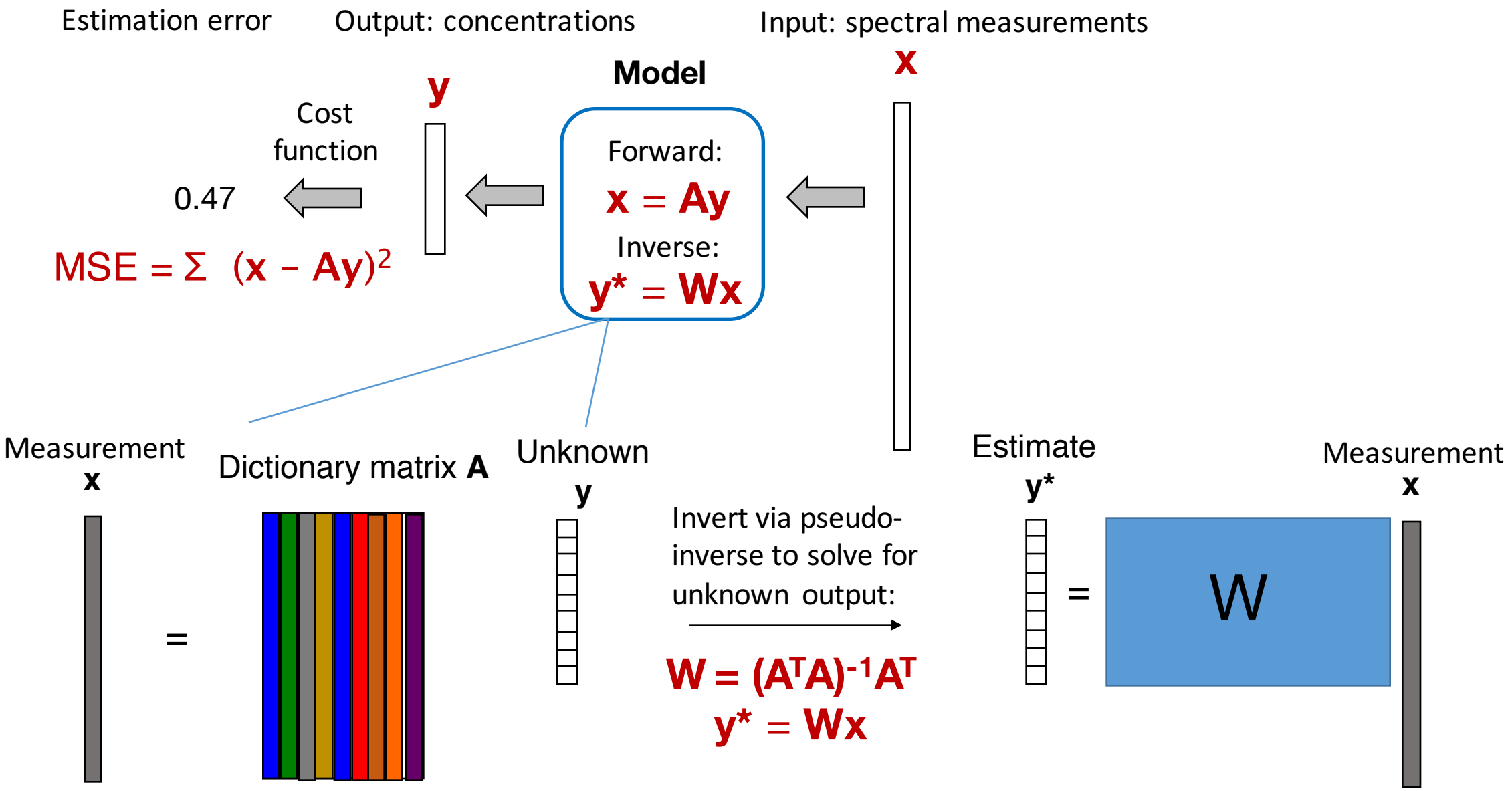

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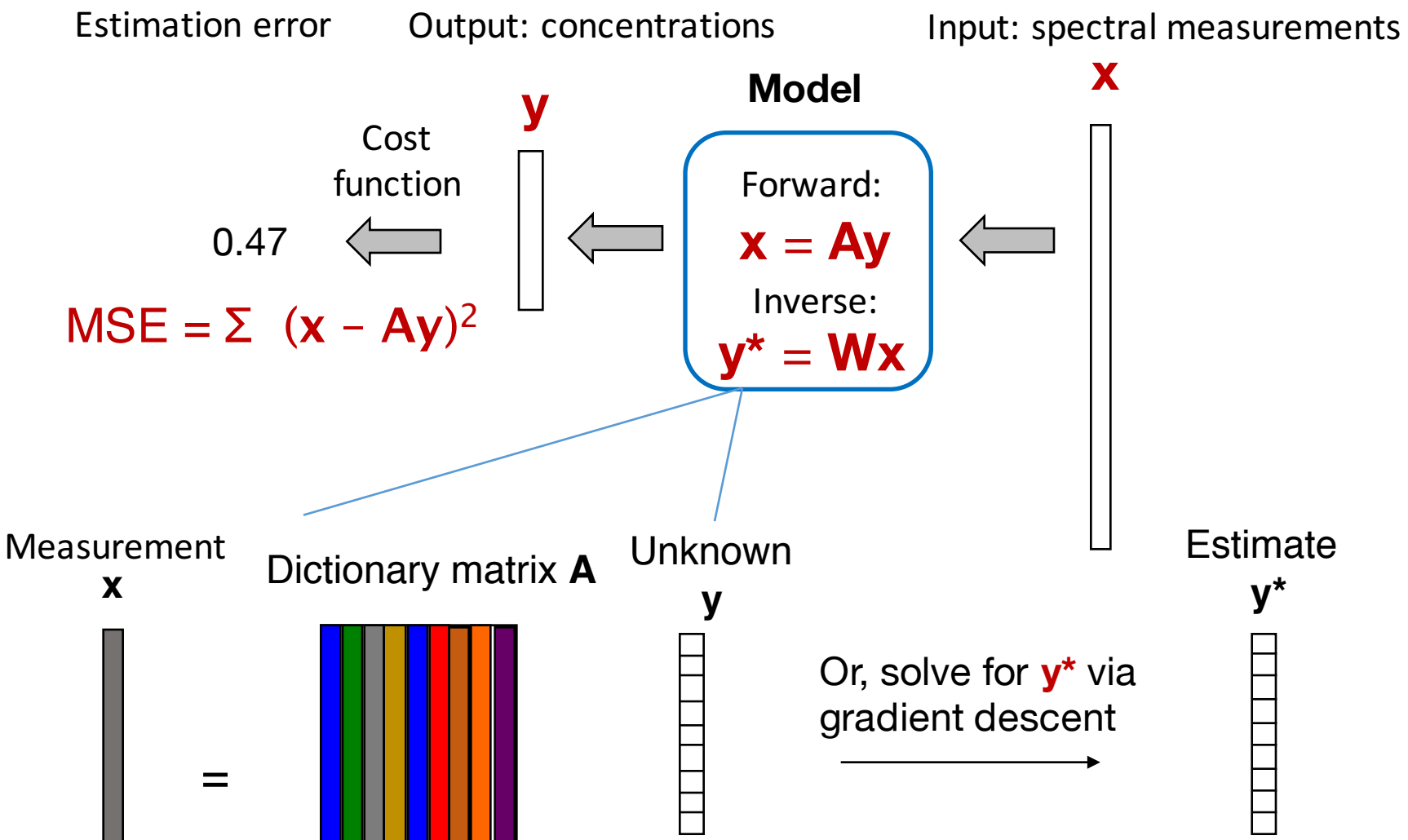
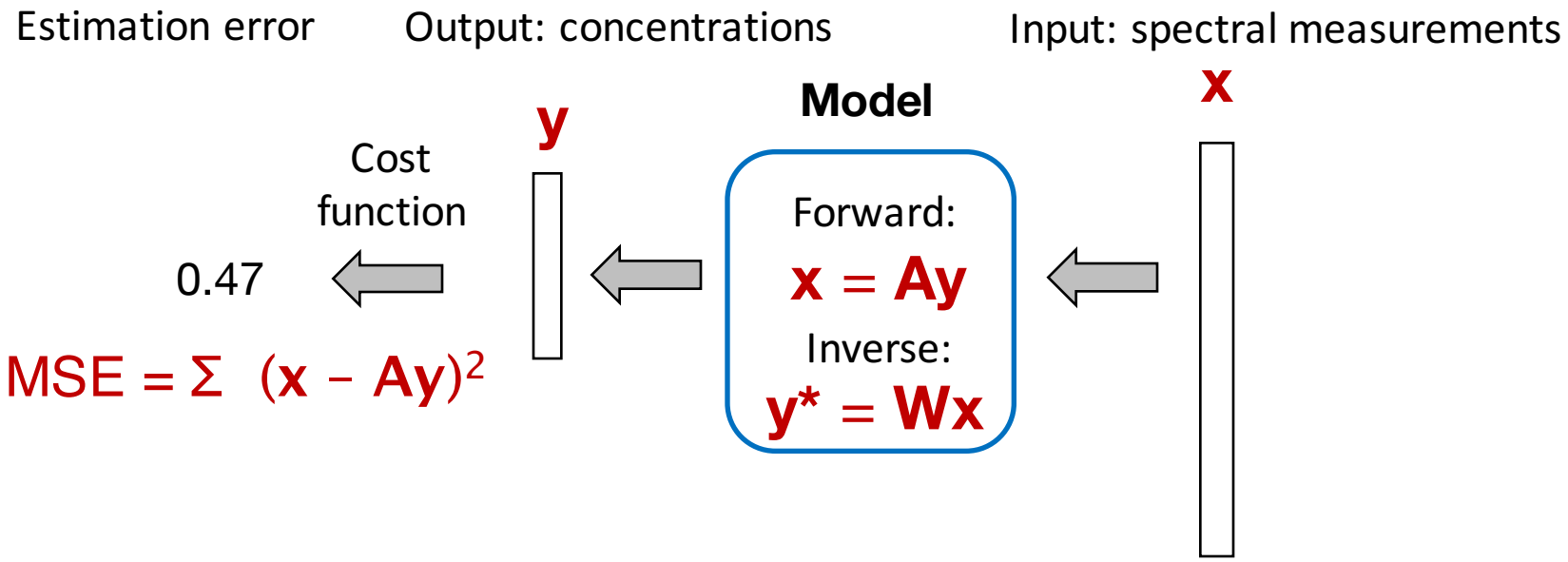
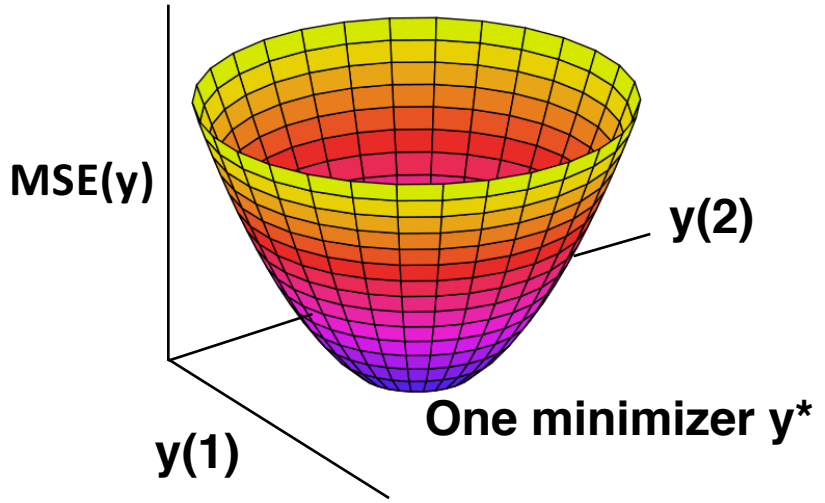


Optimization pipeline for spectral unmixing



$$MSE(\mathbf{y}) = \sum_{\text{spectral measurements}} (\mathbf{x} - \mathbf{A}\mathbf{y})^2$$

$$d/d\mathbf{y}\ MSE = \mathbf{A}^T(\mathbf{x} - \mathbf{A}\mathbf{y})$$



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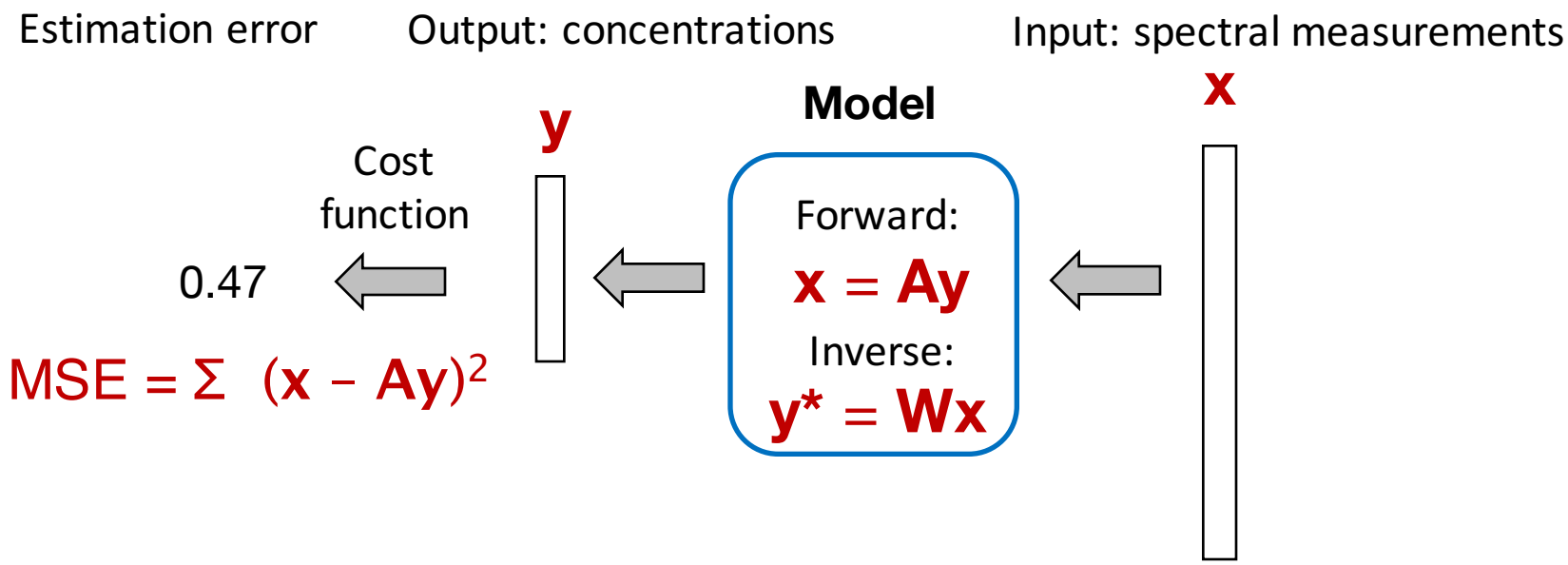

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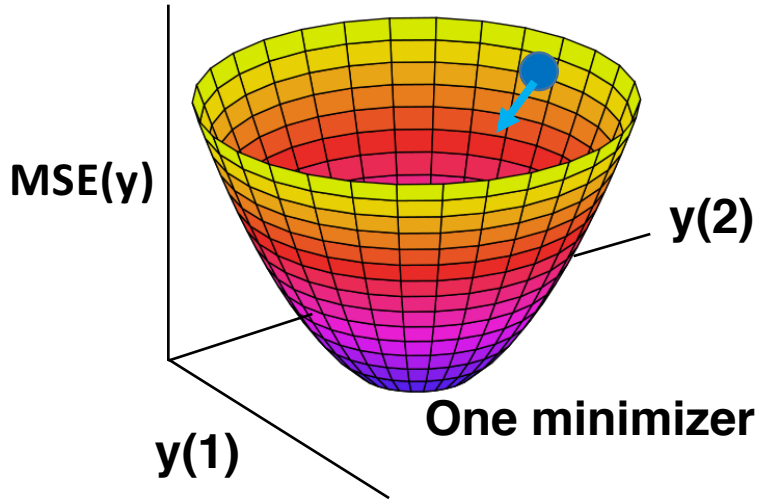
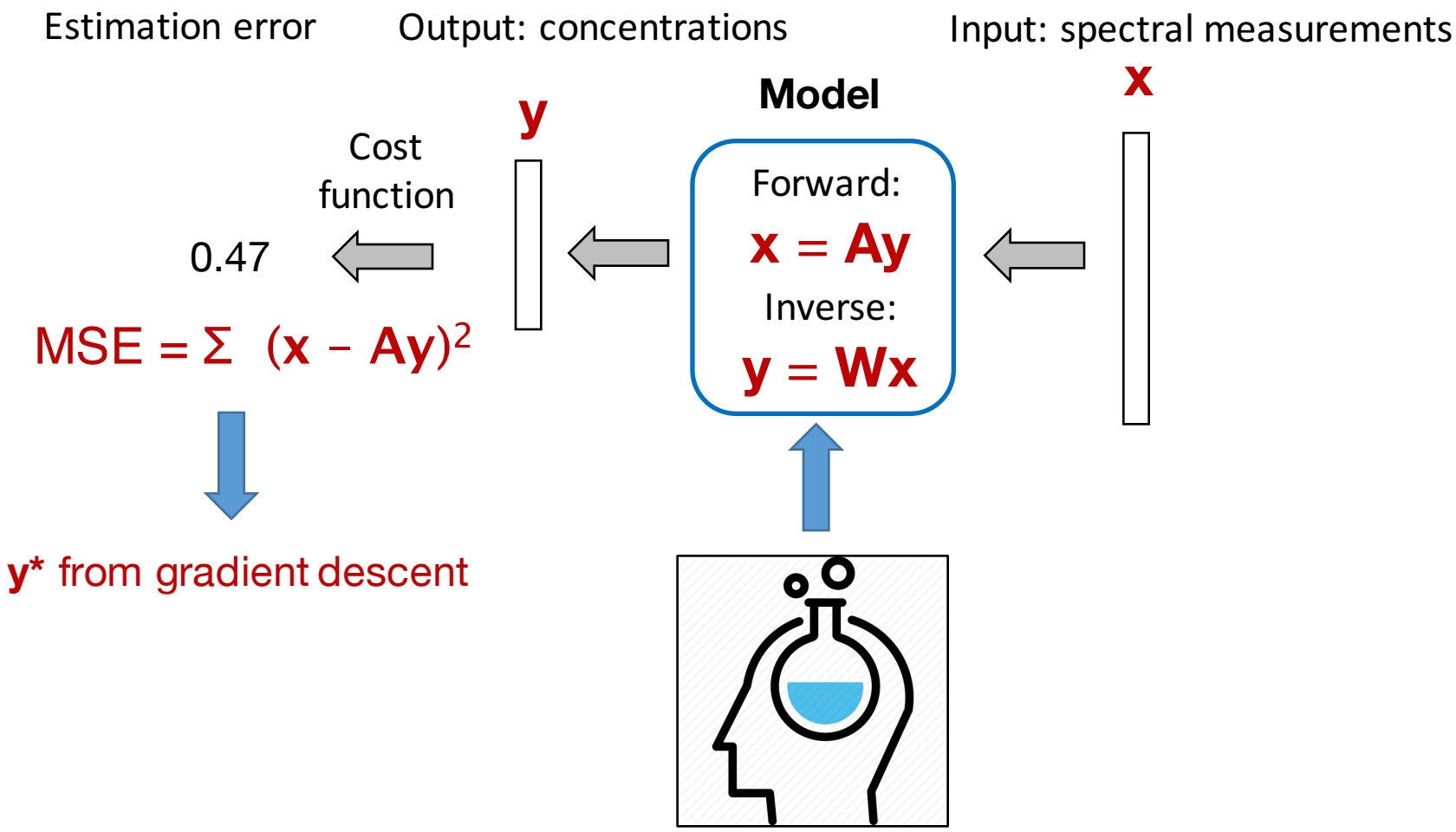


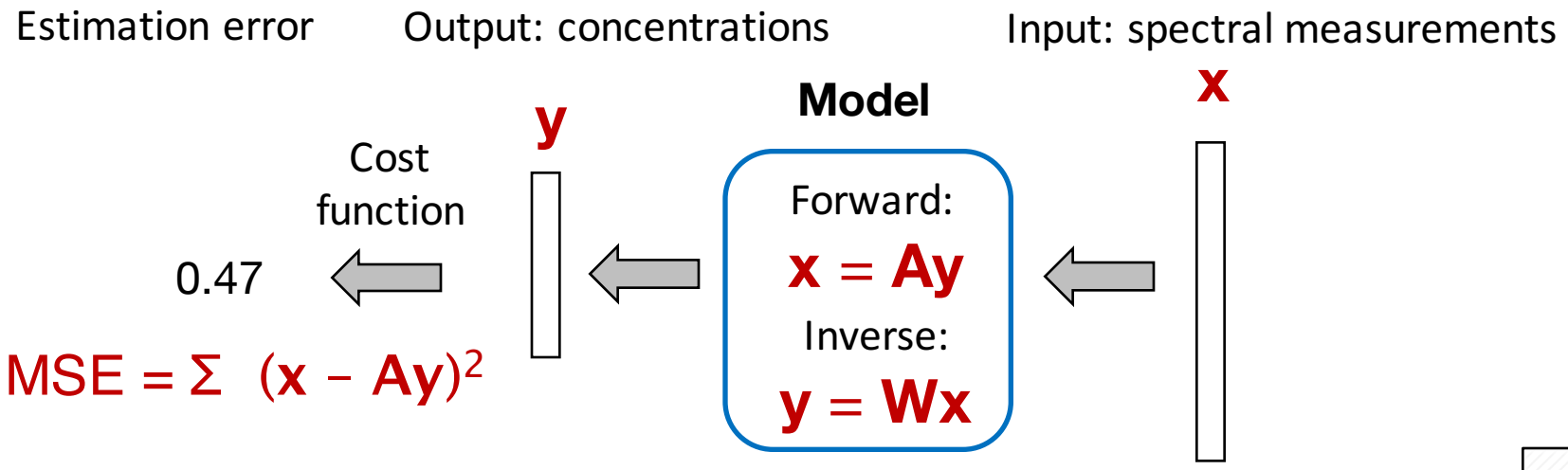
1. Guess output **y**
2. Evaluate slope
3. If its large, take a step:

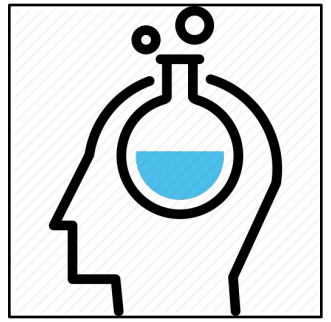
$$\mathbf{y} - \mathbf{y} + \varepsilon\mathbf{A}^T(\mathbf{x} - \mathbf{A}\mathbf{y})$$

Optimization pipeline for spectral unmixing



Optimization pipeline for spectral unmixing

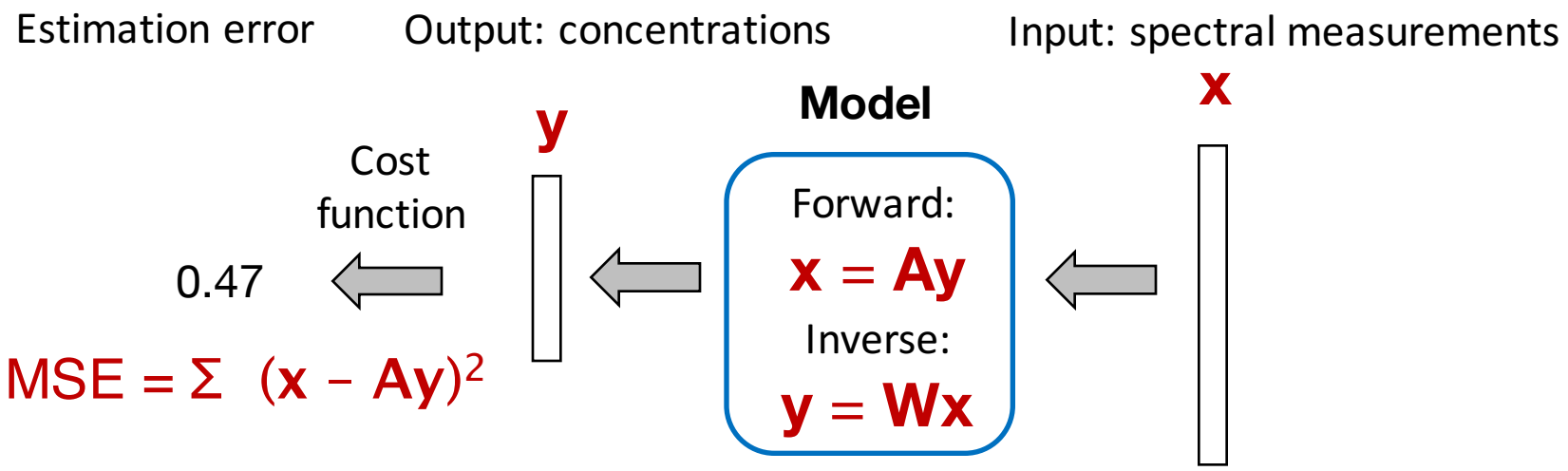




A and **W** from first principles

Optimization: You only care about finding the best solution **y***

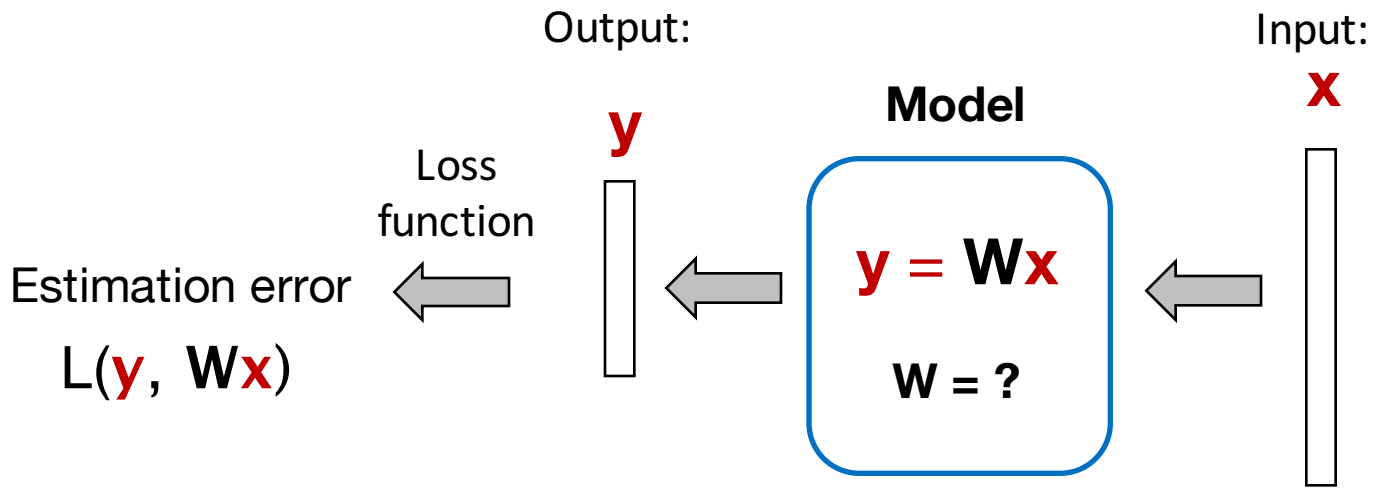
Optimization pipeline for spectral unmixing



Optimization: You only care about finding the best solution **y***

Machine Learning: You first care about finding the model **W**, then you'll use that to find the best solution **y***

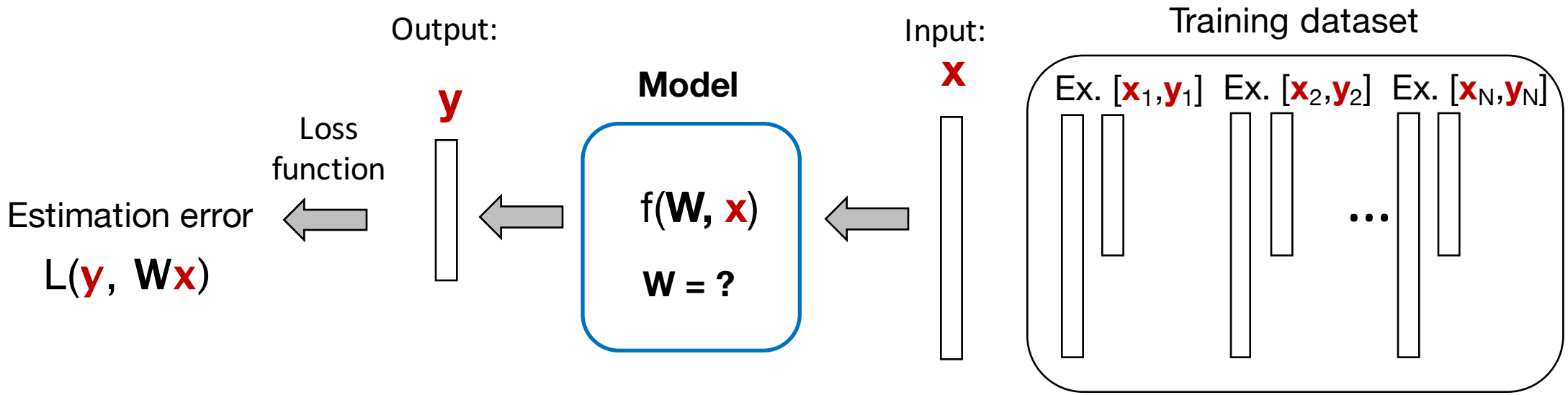
Pipeline for machine learning



Changes for machine learning framework:

1. Now just establish the mapping from inputs to outputs (here, matrix **W**)

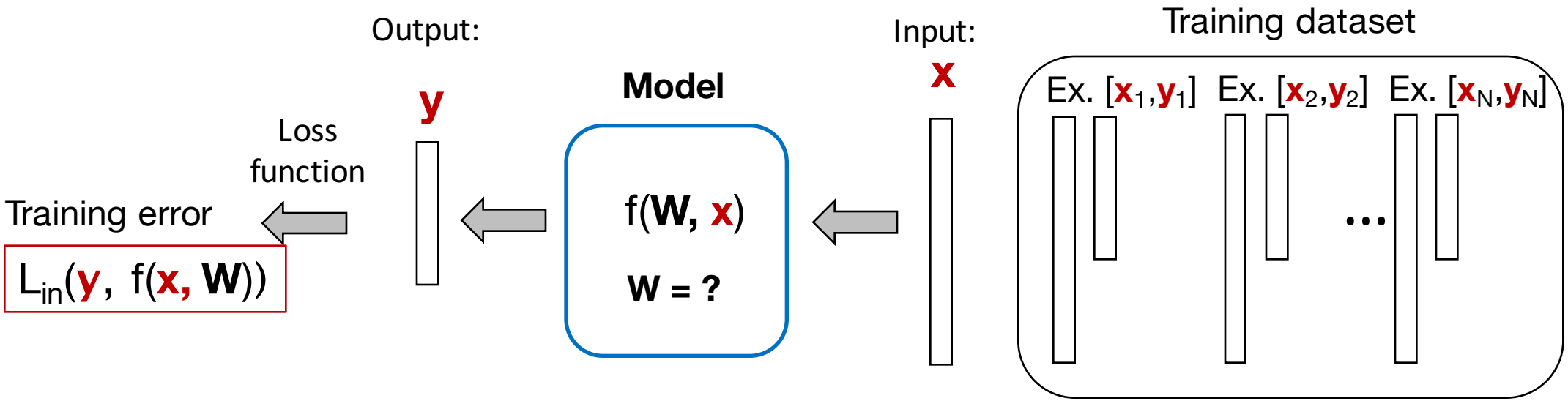
Pipeline for machine learning



Changes for machine learning framework:

1. Now just establish the mapping from inputs to outputs (here, matrix **W**)
2. Must first determine mapping f(**x,** **W**) using large set of "training" data

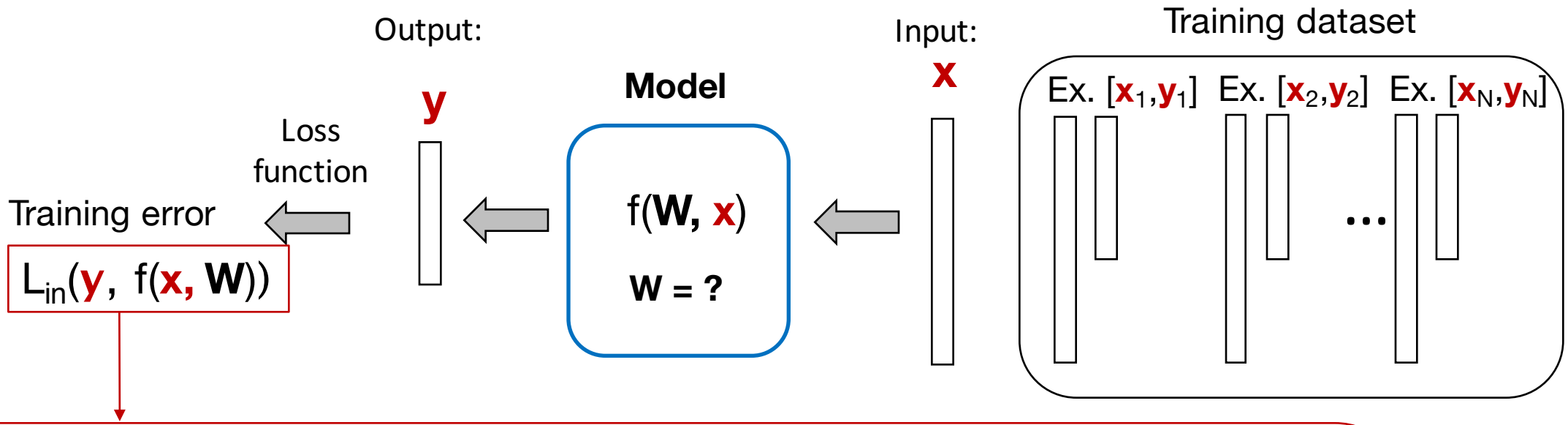
Pipeline for machine learning



Changes for machine learning framework:

1. Now just establish the mapping from inputs to outputs (here, matrix **W**)
2. Must first determine mapping f(**x**, **W**) using large set of "training" data
3. Use a *loss function* L that depends upon the training inputs (x,y) *and* the model (**W**)

Pipeline for machine learning

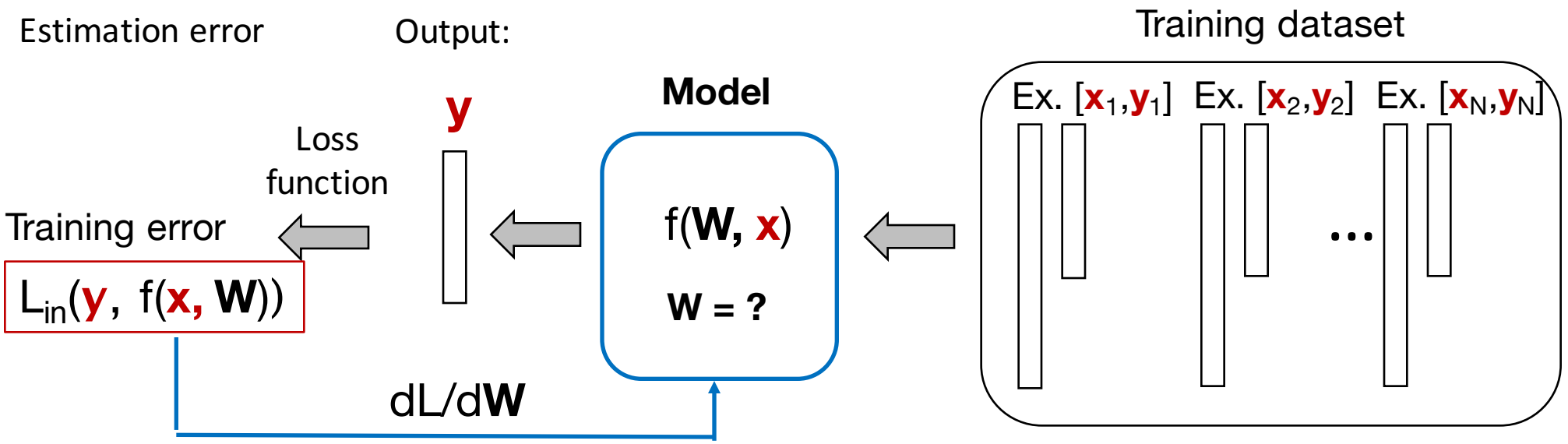


Training Error ("in class error"):

- L_{in} compares modeled output, $f(\mathbf{x}_i, \mathbf{W})$, with the *correct* output that has been *labeled*
- Assume error caused by each labeled example is equally important and sum them up:

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, \mathbf{W}), y_i)$$

Pipeline for machine learning



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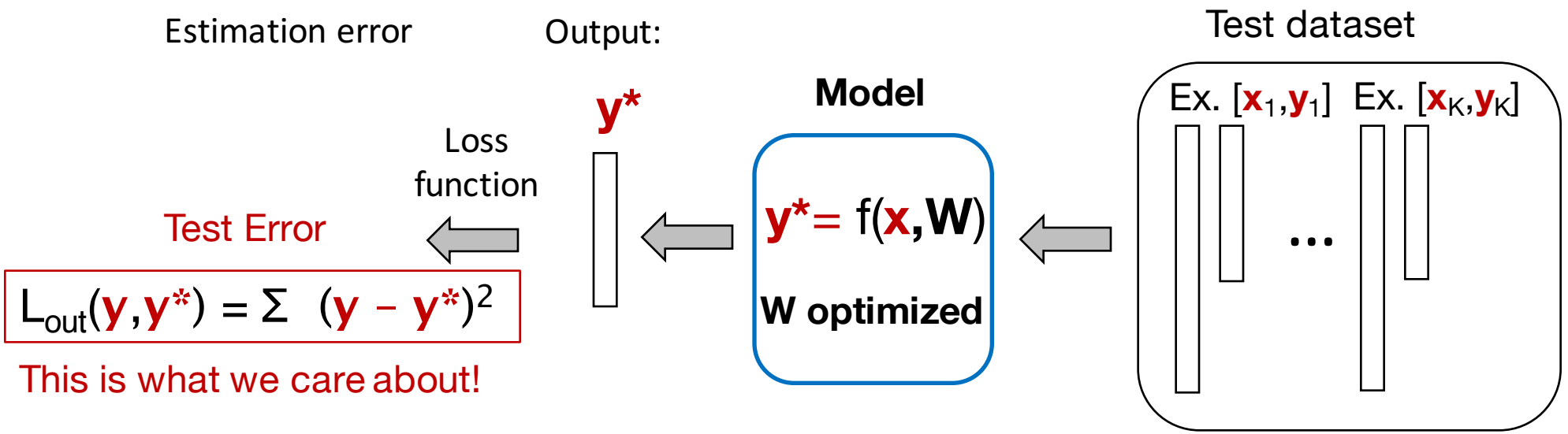
4. Find optimal mapping (**W**), using the training data to guide gradient descent on L

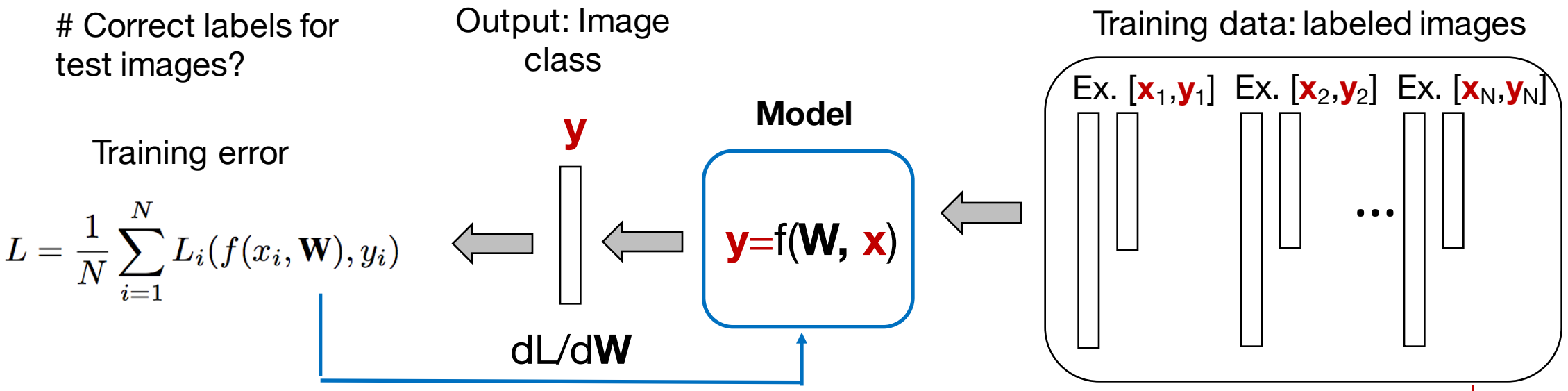
Pipeline for machine learning



Changes for machine learning framework:

1. Now just establish the mapping from inputs to outputs (here, matrix **W**)
2. Must first determine mapping (**W**) using large set of "training" data
3. Use a *loss function* L(**x**,**W**) that depends upon the inputs x *and* the model (**W**)
4. Find optimal mapping (**W**), using the training data to guide gradient descent on L
5. Then evaluate model accuracy by sending *new* **x** through and comparing output **y*** to "test" data **y**

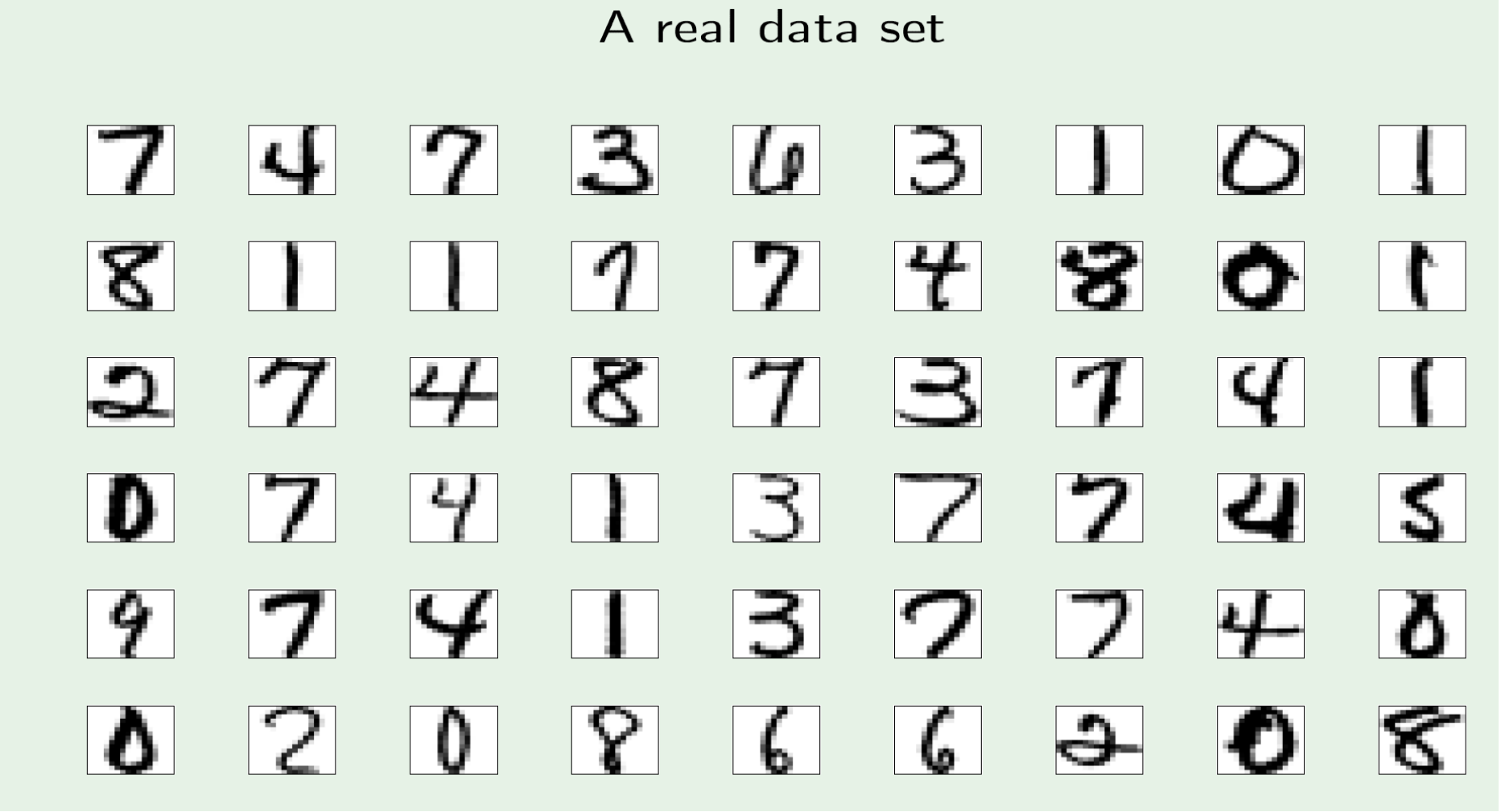
Example: machine learning for image classification



Let's consider a simple example – image classification. What do we need for training?

1. Labeled examples $\{(x_i, y_i)\}_{i=1}^{N}$

Example: machine learning for image classification

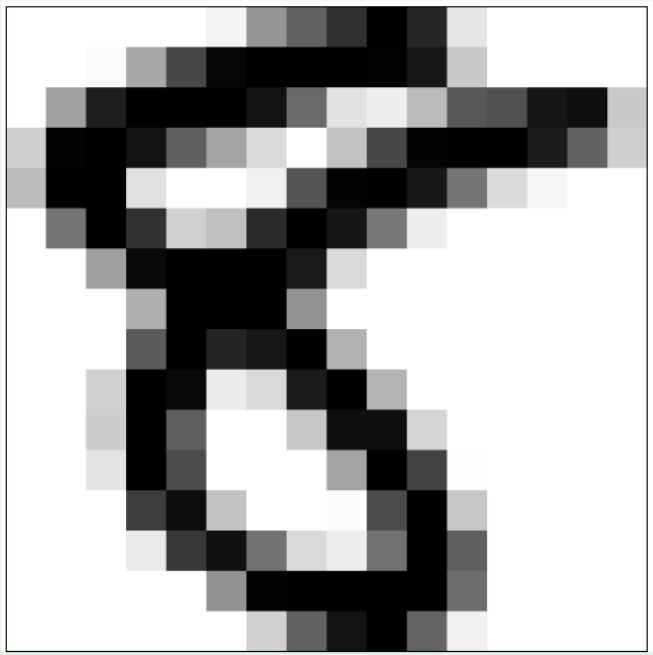


From Yaser Abu Mustafa, Machine Learning course at Caltech

Input representation

'raw' input $\mathbf{x} = (x_0, x_1, x_2, \cdots, x_{256})$

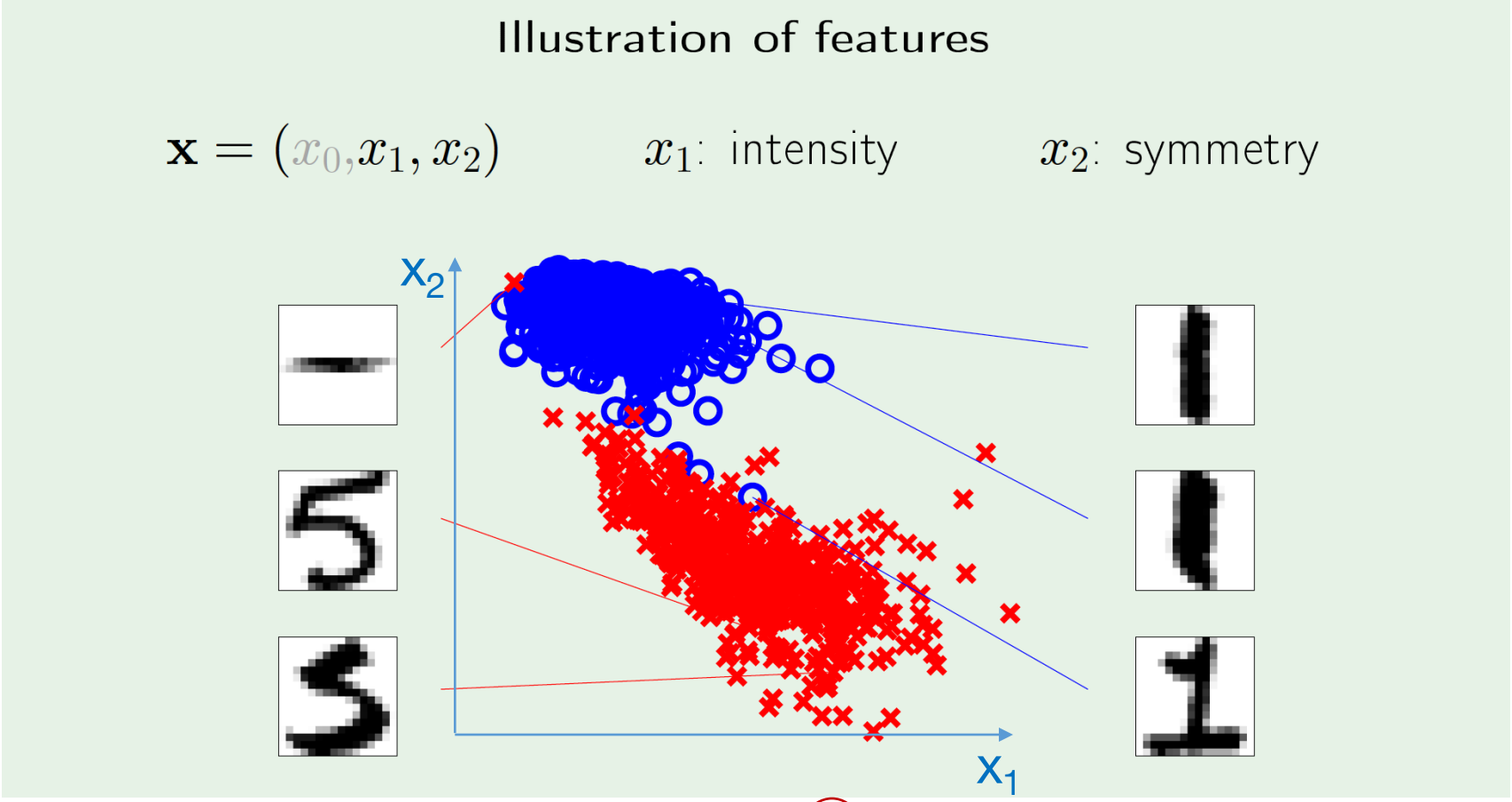
linear model: $(w_0, w_1, w_2, \cdots, w_{256})$



Features: Extract useful information, e.g.,

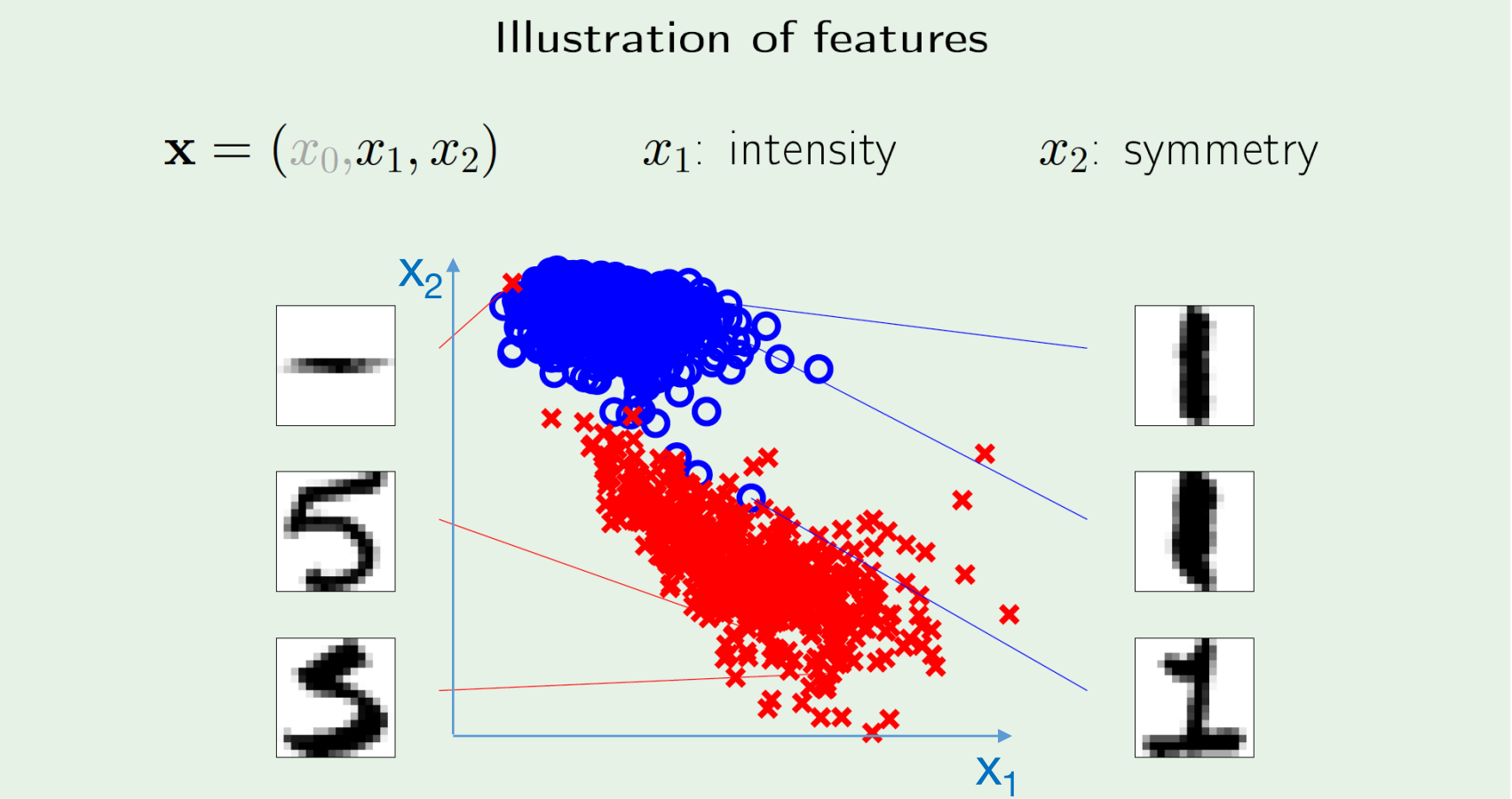
intensity and symmetry $\mathbf{x} = (x_0, x_1, x_2)$

linear model: (w_0, w_1, w_2)



Dataset: 1000 examples of 1's and 5's mapped to $\mathbf{x_j} = (1, x_1, x_2)$, with associated label $y_j = 1$ or -1

This transforms wx+b into **wx**



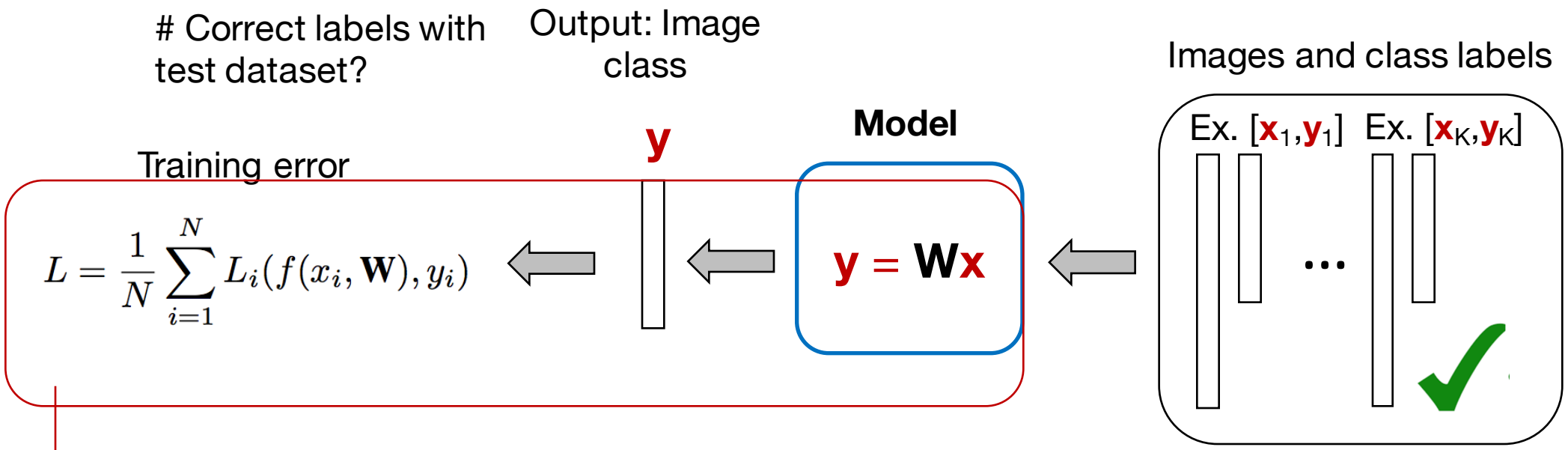
Dataset: 1000 examples of 1's and 5's mapped to $\mathbf{x}_j = (1, x_1, x_2)$, with associated label $y_j = 1$ or -1

$[\mathbf{X}_{train}, \mathbf{Y}_{train}] = [\mathbf{x}_j, \mathbf{y}_j]$ for n=1 to 750 $[\mathbf{X}_{test}, \mathbf{Y}_{test}] = [\mathbf{x}_j, \mathbf{y}_j]$ for n=751 to 1000

Labeled data:

Training dataset	Test dataset
n=1-750	n=751-1000

Example: machine learning for image classification



Let's consider a simple example – image classification. What do we need for training?

✓ **1. Labeled examples** $\{(x_i, y_i)\}_{i=1}^{N}$

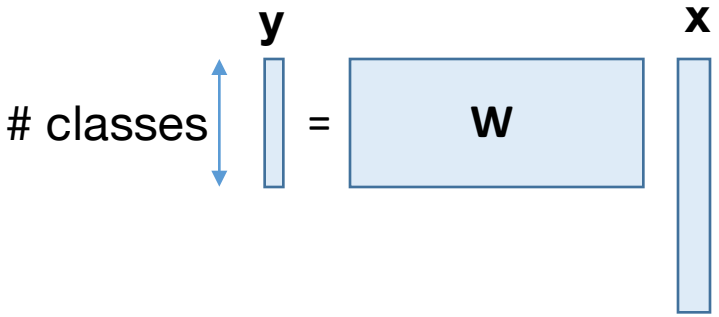
2. A model and loss function

Let's start with a simpler approach: linear regression

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, \mathbf{W}), y_i)$$

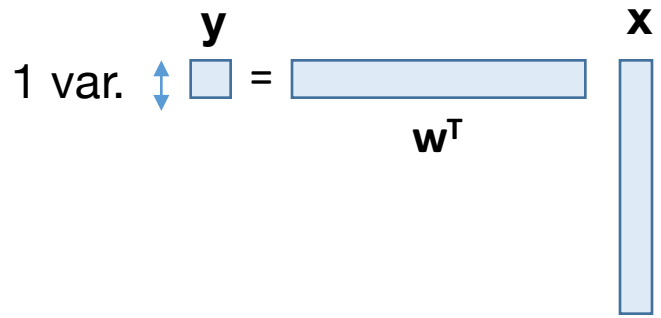
General linear model:

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(\mathbf{W}\mathbf{x}_i, y_i)$$



Assume 1 class = 1 linear fit

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(w^T x_i - y_i)$$



Use MSE error model

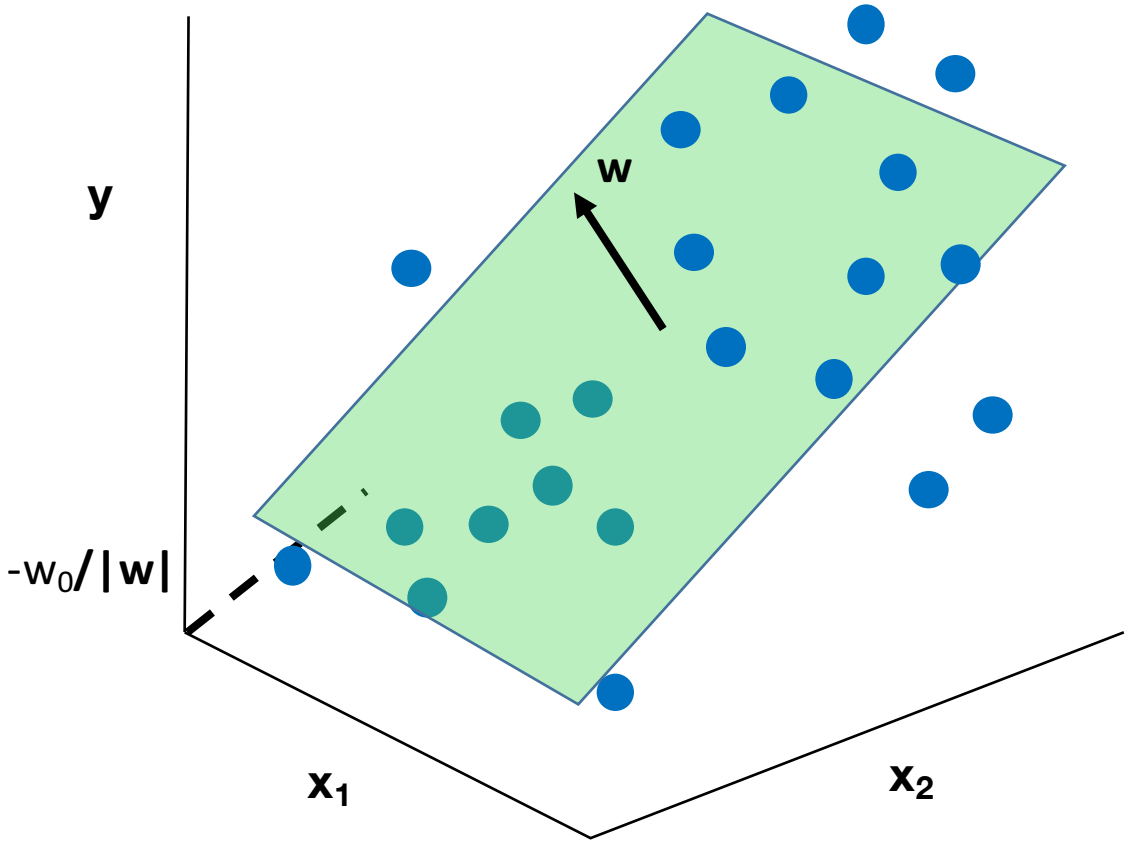
$$L = \frac{1}{N}\sum_{i=1}^{N} (w^T x_i - y_i)^2$$

Where labels determined by thresholding

$$f(\mathbf{x}_i) = y_i^* = \text{sgn}(\mathbf{w}^T\mathbf{x}_i)$$

$$\text{sgn}(x) := \begin{cases} -1 & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ 1 & \text{if } x > 0. \end{cases}$$

Why does linear regression with sgn() achieve classification?



Without sgn(): regression for best fit

$$f(\mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i$$

$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

- If y_i can be anything, minimizing *L* makes **w** the plane of best fit

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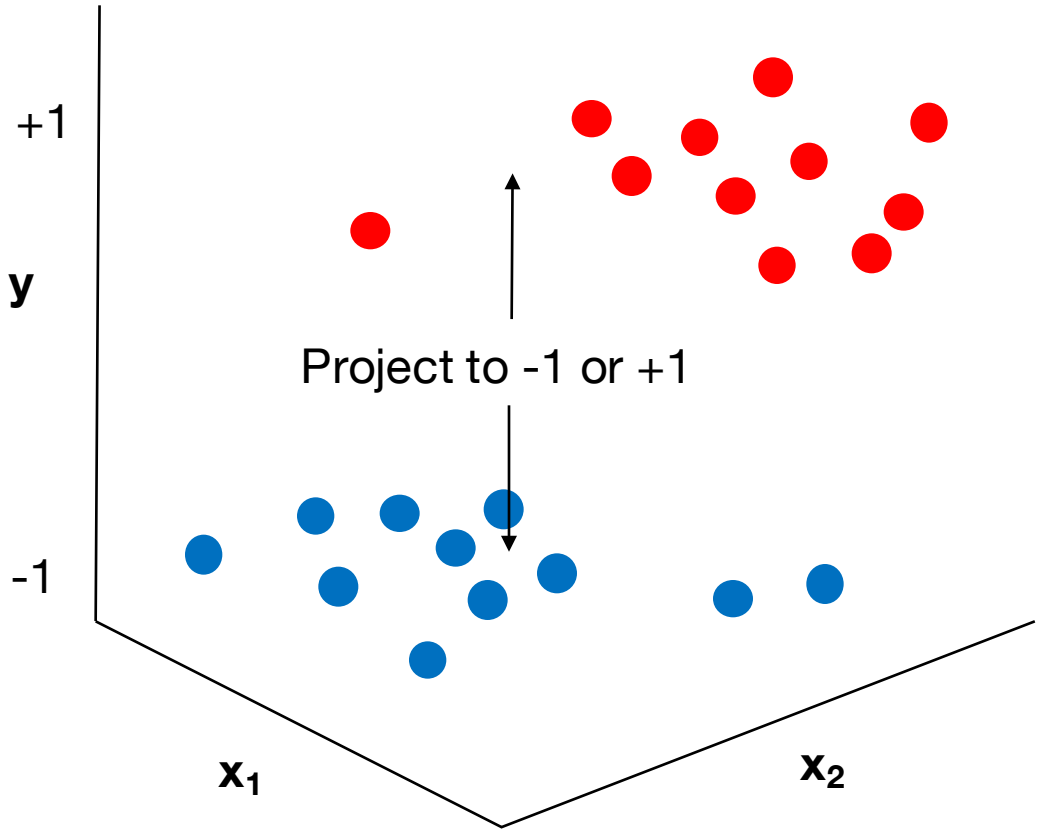

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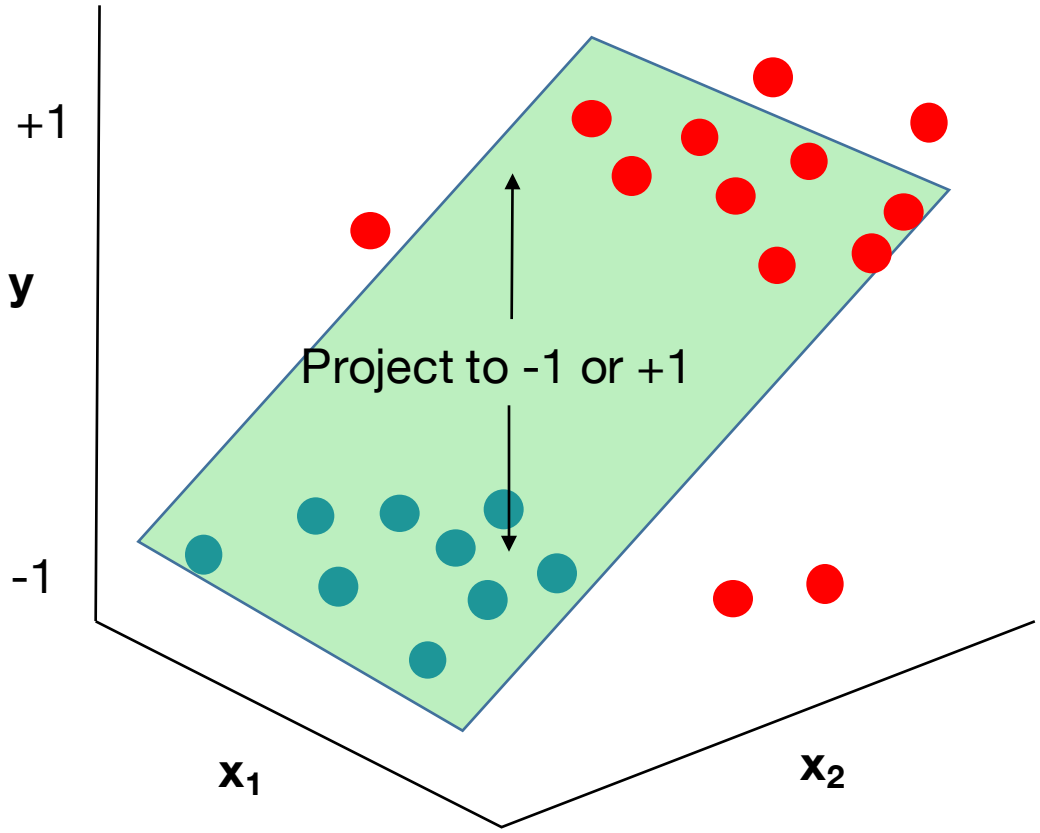

Without sgn(): regression for best fit

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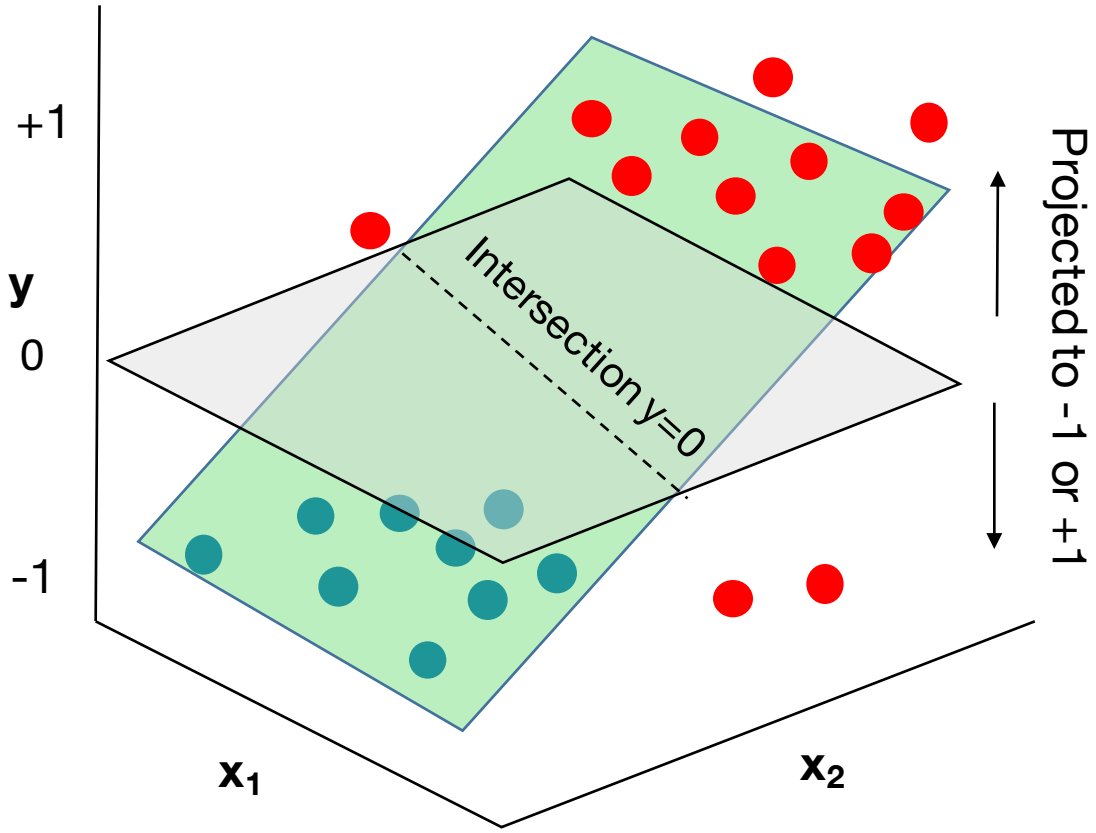
$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

- y_i can only be -1 or +1, which defines its class
- Can still find plane of best fit

Why does linear regression with sgn() achieve classification?



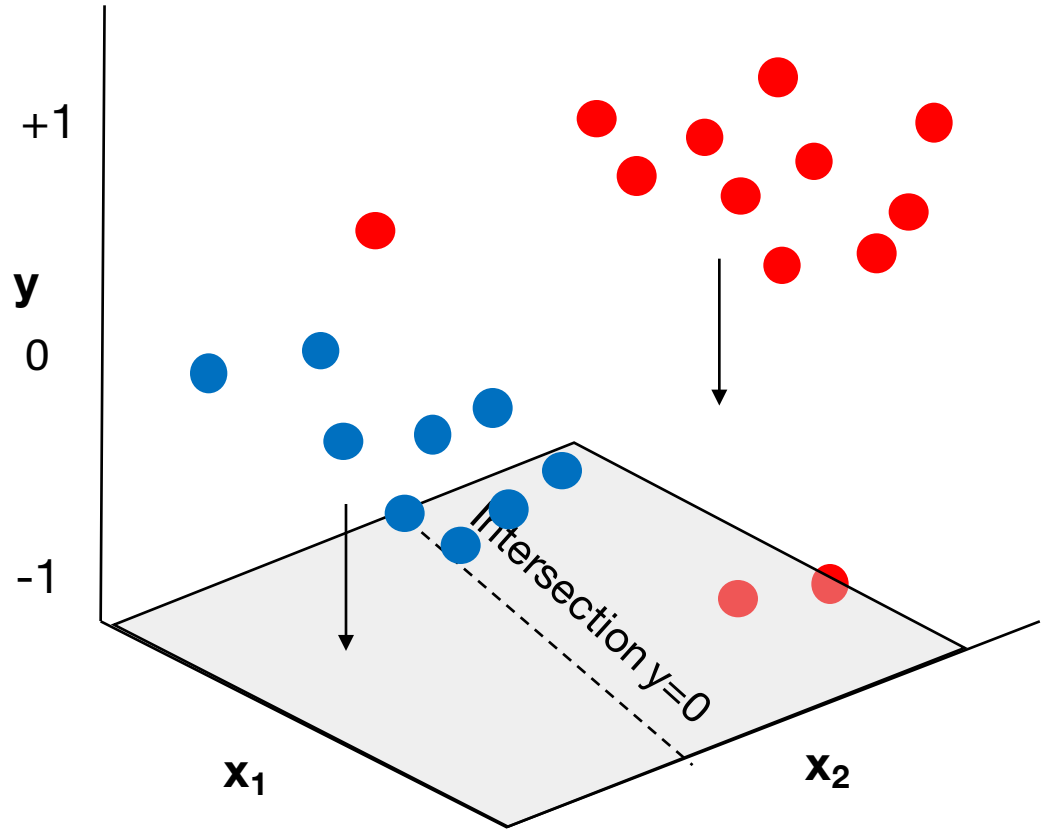
With sgn() operation:

$$f(\mathbf{x}_i) = y_i^* = \text{sgn}(\mathbf{w}^T\mathbf{x}_i)$$

$$L = \frac{1}{N}\sum_{i=1}^{N}(w^T x_i - y_i)^2$$

- Anything point to one side of y=0 intersection is class +1, anything on the other side of intersection is class -1

Why does linear regression with sgn() achieve classification?



With sgn() operation:

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$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

- y axis isn't really needed now & can view this decision boundary in 2D

Why does linear regression with sgn() achieve classification?

With sgn() operation:

$$f(\mathbf{x}_i) = y_i^* = \text{sgn}(\mathbf{w}^T \mathbf{x}_i)$$

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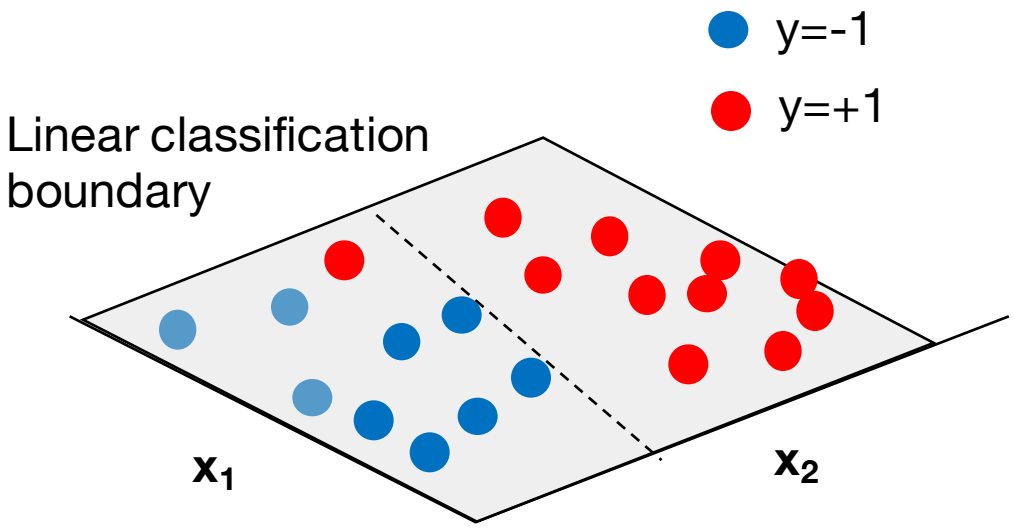
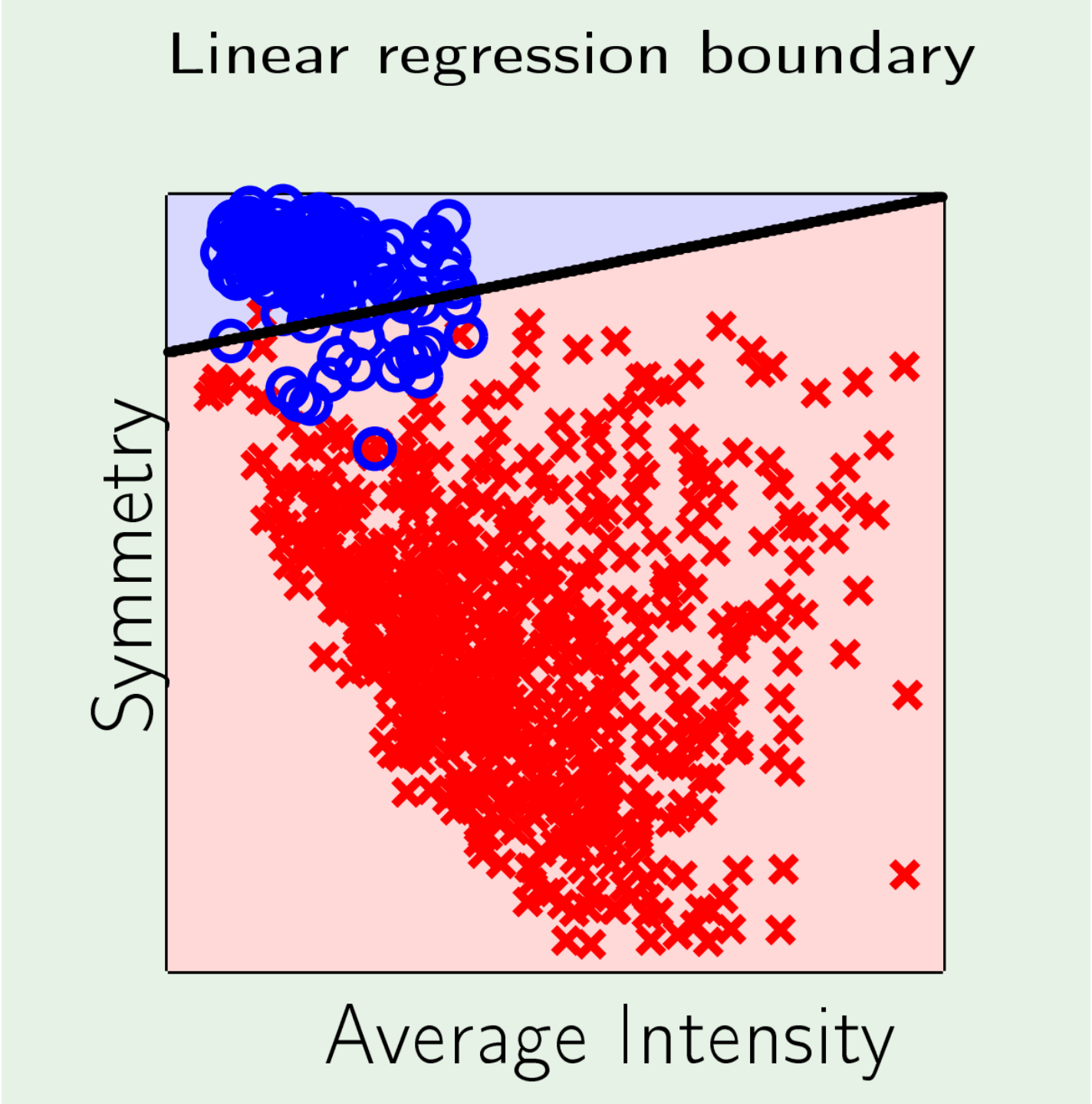
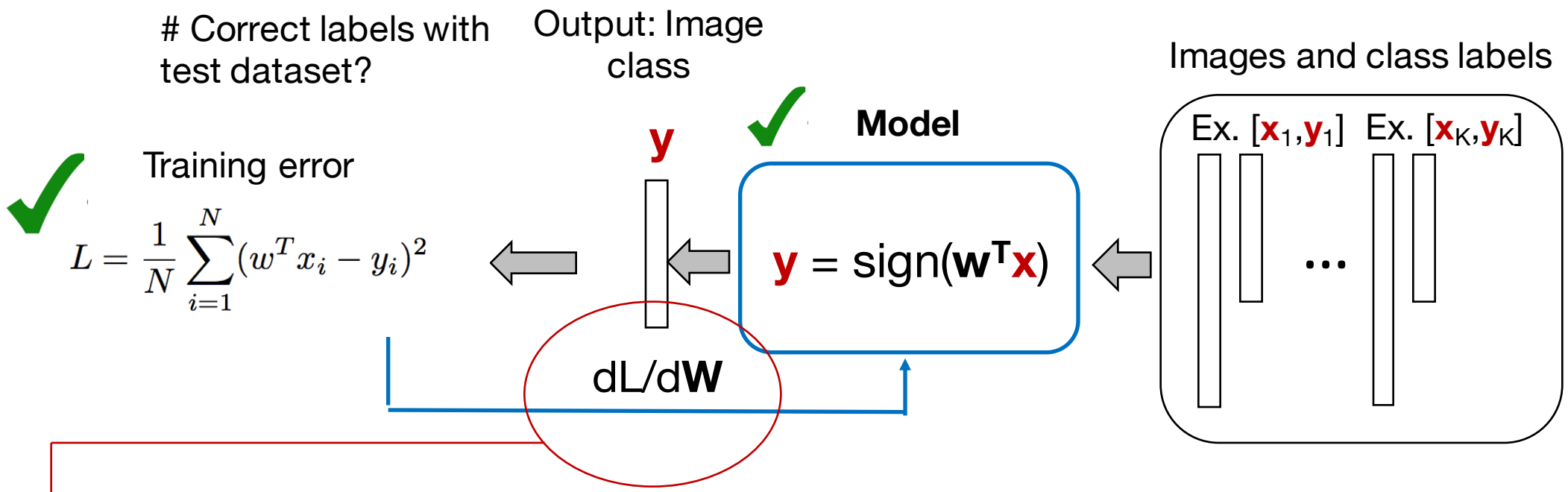


Sign operation takes linear regression and makes it a classification operation!


Linear regression boundary
Symmetry
Average Intensity

Example: machine learning for image classification



Let's consider a simple example – image classification. What do we need for training?

1. **Labeled examples**
2. **A model and loss function**
3. **A way to minimize the loss function L**

3 methods to solve for w^T in the case of linear regression:

(easier)

1. Pseudo-inverse (this is one of the few cases with a closed-form solution)
2. Numerical gradient descent
3. Gradient descent on the cost function with respect to W

(harder)

$$L(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - y_n\right)^2$$

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$$= \frac{1}{N}\|\mathrm{X}\mathbf{w} - \mathbf{y}\|^2$$

where $\mathrm{X} = \begin{bmatrix} —\mathbf{x}_1{}^{\mathsf{T}}— \\ —\mathbf{x}_2{}^{\mathsf{T}}— \\ \vdots \\ —\mathbf{x}_N{}^{\mathsf{T}}— \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$

Write this out as a matrix equation:

$$L = \frac{1}{N} \|Xw - y\|^2$$

Note: Training data goes into “dictionary” matrix

$$L = \frac{1}{N} \left(w^T X^T X w - 2 w^T X^T y + y y^T \right)$$

Take derivative wrt w and set to 0:

$$\nabla L(w) = \frac{2}{N} X^T (Xw - y) = 0$$

Solution is pseudo-inverse:

$$w_o = (X^T X)^{-1} X^T y$$

The linear regression algorithm

1: Construct the matrix $\mathbf{X}$ and the vector $\mathbf{y}$ from the data set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$ as follows

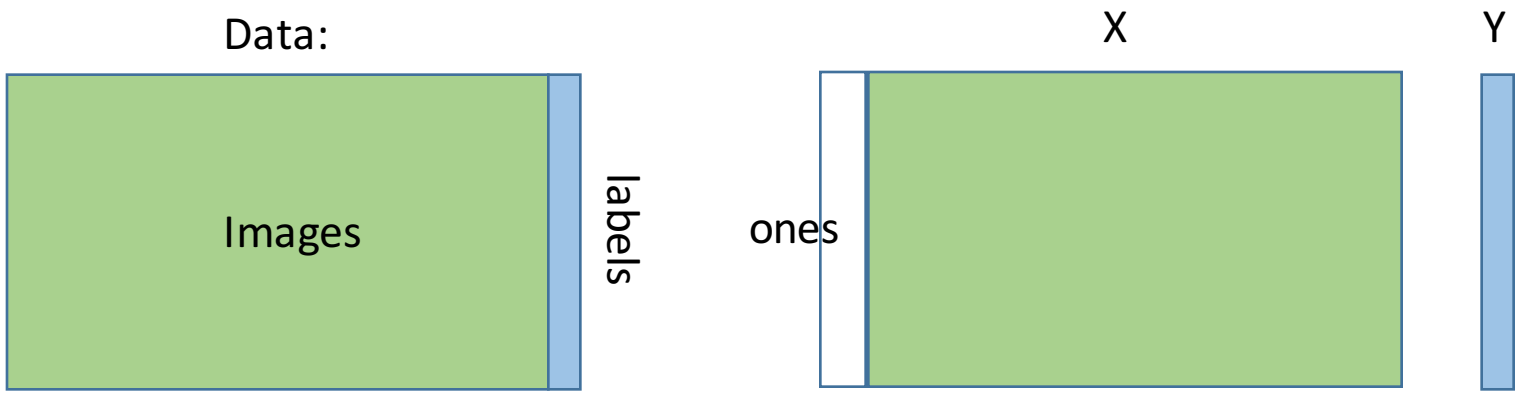
$$\underbrace{\mathbf{X} = \begin{bmatrix} —\mathbf{x}_1^\mathsf{T}— \\ —\mathbf{x}_2^\mathsf{T}— \\ \vdots \\ —\mathbf{x}_N^\mathsf{T}— \end{bmatrix}}_{\text{input data matrix}}, \qquad \underbrace{\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}}.$$

2: Compute the pseudo-inverse $\mathbf{X}^\dagger = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}$.

3: Return $\mathbf{w} = \mathbf{X}^\dagger\mathbf{y}$.

Example pseudo-code

```
data = np.loadtxt('train_data.txt', dtype=int)
X = numpy.zeros((data.shape[0],data.shape[1]-1))
X[:,0]=1
Y = numpy.zeros((data.shape[0],1))
for row in m:
    X[row,1:X.shape[1]-1] = data[row,0:data.shape[1]:1]
    Y[row] = data[row,data.shape[1]-1]
X_dagger = np.linalg.pinv(X)
w = np.matmul(X_dagger,Y)
```



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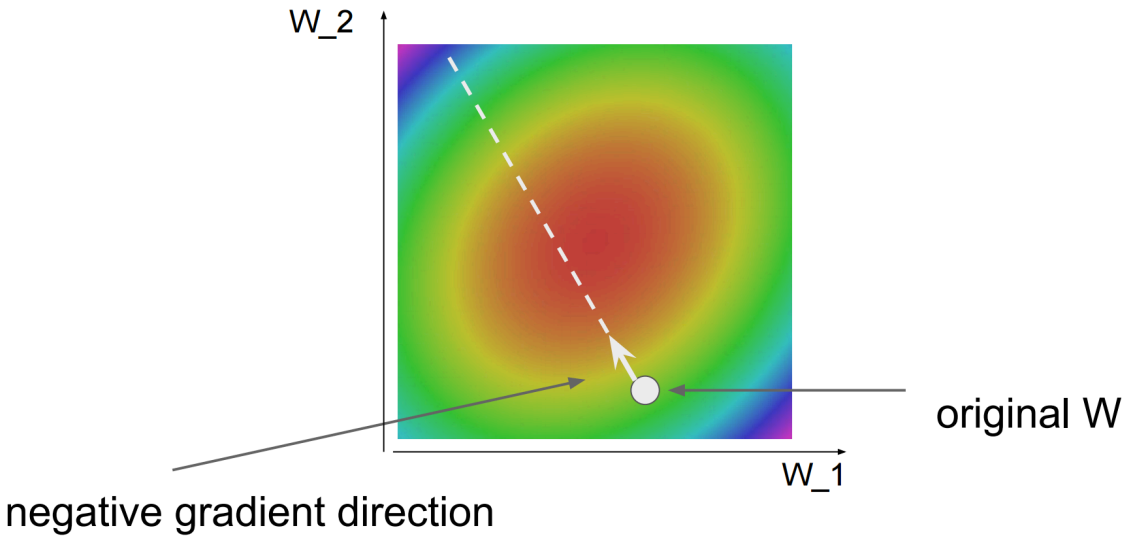
Gradient descent: The iterative recipe

Initialize: Start with a guess of **W**

Until the gradient does not change very much:
dL/d**W** = evaluate_gradient(**W**, **x** ,y ,L)
W = **W** – step_size * dL/d**W**

evaluate_gradient can be achieved numerically or algebraically



Gradient descent: Numerical evaluation example

With a matrix, compute this for each entry:

$$\frac{dL(W_i)}{dW_i} = \lim_{h \to 0} \frac{L(W_i + h) - L(W_i)}{h}$$

Example:

W = [1,2;3,4]
L(W, x, y) = 12.79

W_1+h = [1.001,2;3,4]
L(W_1+h, x, y) = 12.8

$dL(W_1)/dW_1$ = 12.8-12.79/.001

$dL(W_1)/dW_1$ = 10

- Repeat for all entries of **W**, dL/d**W** will have NxM entries for NxM matrix

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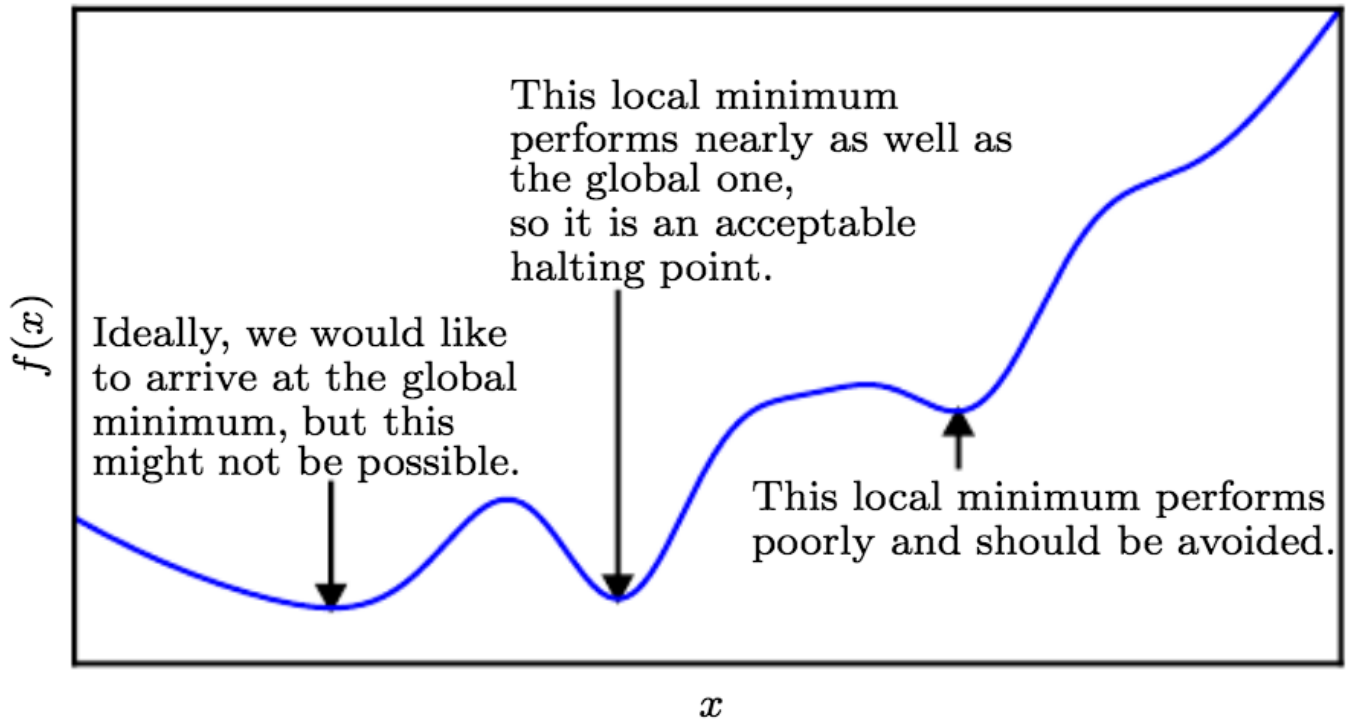
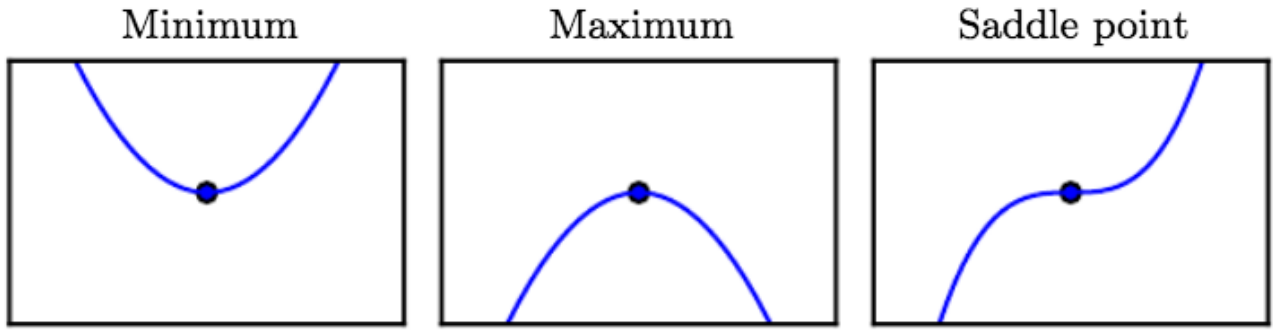
(harder)

Some quick details about gradient descent

- For non-convex functions, local minima can obscure the search for global minima
- Analyzing critical points (plateaus) of function of interest is important
- Critical points at $df/dx = 0$
- 2nd derivative d^2f/dx^2 tells us the type of critical point:
  - Minima at $d^2f/dx^2 > 0$
  - Maxima at $d^2f/dx^2 < 0$





Some quick details about gradient descent

Often we'll have functions of m variables

$f : \mathbb{R}^n \to \mathbb{R}$ (e.g., f(**x**) = Σ (**Ax-y**)^2)

Will take partial derivatives $\frac{\partial}{\partial x_i} f(\boldsymbol{x})$ and put them in gradient vector **g:** $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$

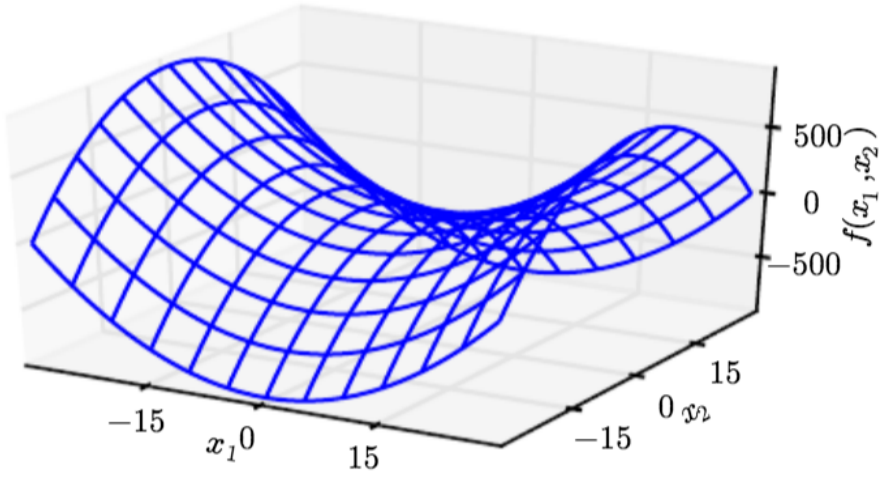
Will have many second derivatives: $\boldsymbol{H}(f)(\boldsymbol{x})_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(\boldsymbol{x})$ Hessian Matrix

In general, we'll have functions that map m variables to n variables

$\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ (e.g., **f**(**x**) = **Wx**, **W** is n x m)

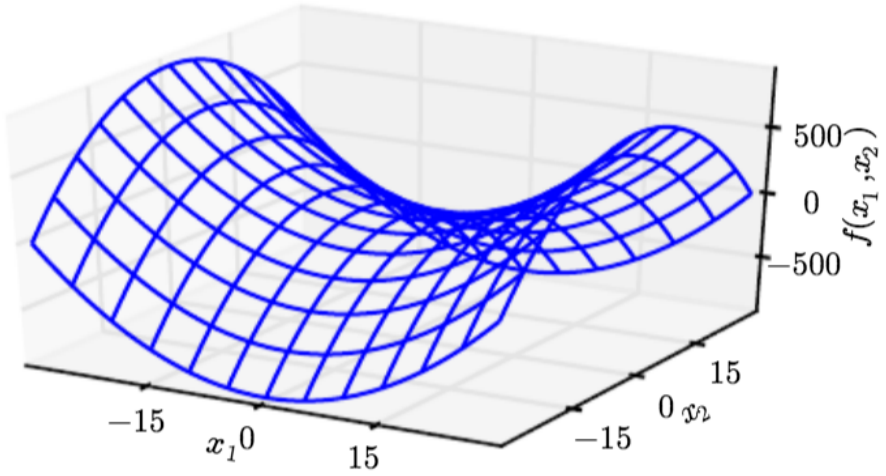
$\boldsymbol{J} \in \mathbb{R}^{n \times m}$ of $\boldsymbol{f}$: $J_{i,j} = \frac{\partial}{\partial x_j} f(\boldsymbol{x})_i$ Jacobian Matrix

Quick example



$$f(\mathbf{x}) = x_1^2 - x_2^2$$

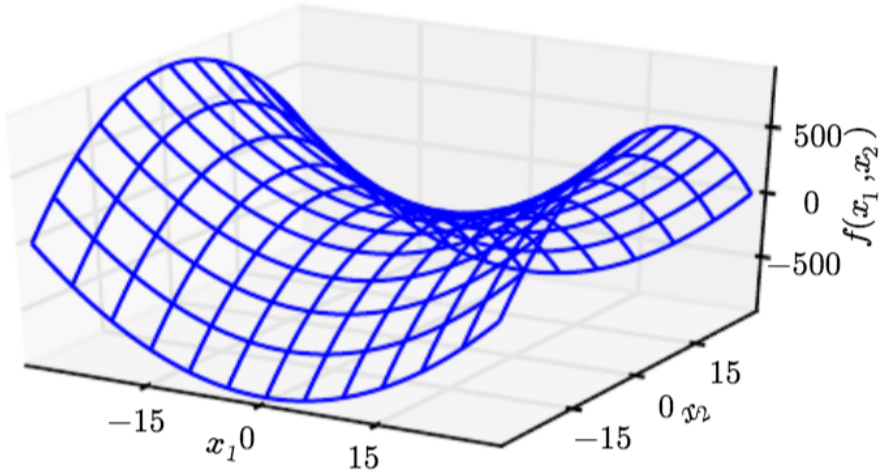
Quick example



$$f(\mathbf{x}) = x_1^2 - x_2^2$$

$$g = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix}$$

Quick example



$$f(\mathbf{x}) = x_1^2 - x_2^2$$

$$g = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix} \qquad H = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

- Convex functions have positive semi-definite Hessians (Trace >= 0)
- Trace/eigenvalues of Hessian are useful evaluate critical points & guide optimization

Steepest descent and the best step size ε

1. Evaluate function $f(\mathbf{x}^{(0)})$ at an initial guess point, $\mathbf{x}^{(0)}$
2. Compute gradient $\mathbf{g}^{(0)} = \nabla_x f(\mathbf{x}^{(0)})$
3. Next point $\mathbf{x}^{(1)} = \mathbf{x}^{(0)} - \boldsymbol{\varepsilon}^{(0)}\mathbf{g}^{(0)}$
4. Repeat – $\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} - \boldsymbol{\varepsilon}^{(n)}\mathbf{g}^{(n)}$, until $|\mathbf{x}^{(n+1)}-\mathbf{x}^{(n)}| <$ threshold t

```
while previous_step_size > precision and iters < max_iters:
    prev_x = cur_x
    cur_x -= gamma * df(prev_x)
    previous_step_size = abs(cur_x - prev_x)
    iters+=1
```

Steepest descent and the best step size ε

What is a good step size $\boldsymbol{\varepsilon}^{(n)}$?

Steepest descent and the best step size ε

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To find out, take 2nd order Taylor expansion of *f* (a good approx. for nearby points):

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}^{(0)}) + (\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \boldsymbol{g} + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^{(0)})^\top \boldsymbol{H}(\boldsymbol{x} - \boldsymbol{x}^{(0)})$$

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Then, evaluate at the next step:

$$f(\boldsymbol{x}^{(0)} - \epsilon \boldsymbol{g}) \approx f(\boldsymbol{x}^{(0)}) - \epsilon \boldsymbol{g}^\top \boldsymbol{g} + \frac{1}{2}\epsilon^2 \boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}$$

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Then, evaluate at the next step:

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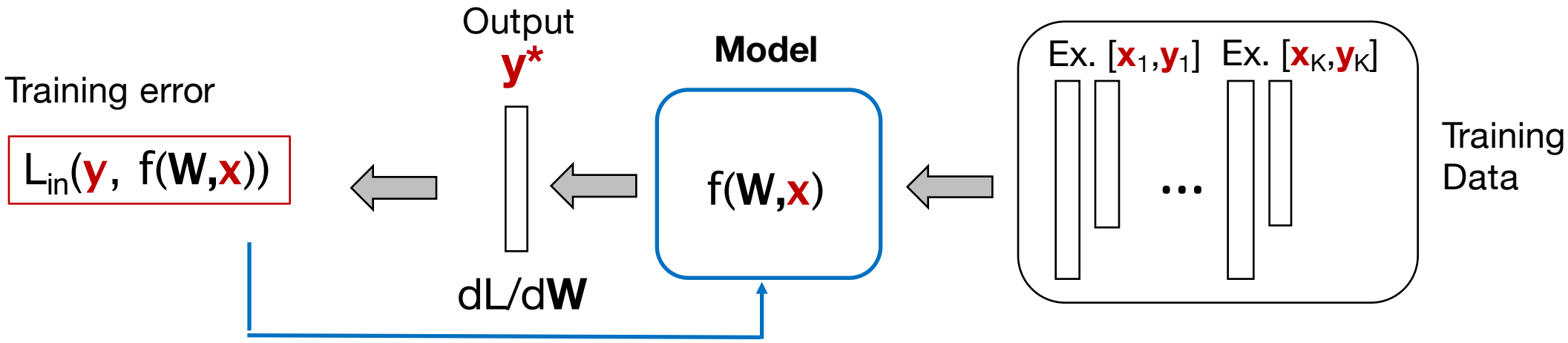
Solve for optimal step (when Hessian is positive): $\boxed{\epsilon^* = \frac{\boldsymbol{g}^\top \boldsymbol{g}}{\boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}}}$

Summary of machine learning pipeline:

1. Network Training

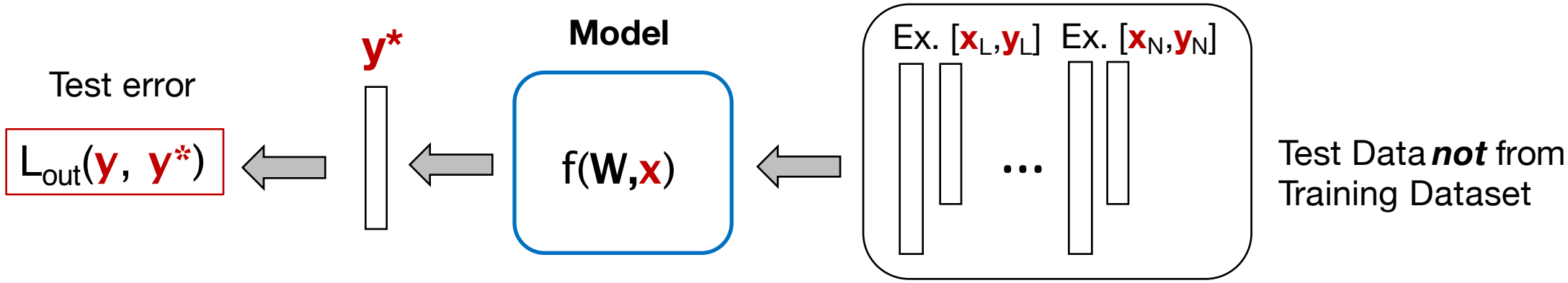


What we need for network training:

1. **Labeled examples**
2. **A model and loss function**
3. **A way to minimize the loss function L**

Summary of machine learning pipeline:

2. Network Testing



What we need for network testing:

4. *Unique* labeled test data
5. Evaluation of model error