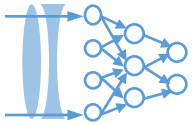


Lecture 6: Ingredients for Machine Learning

Machine Learning and Imaging

BME 590L
Roarke Horstmeyer

Outline

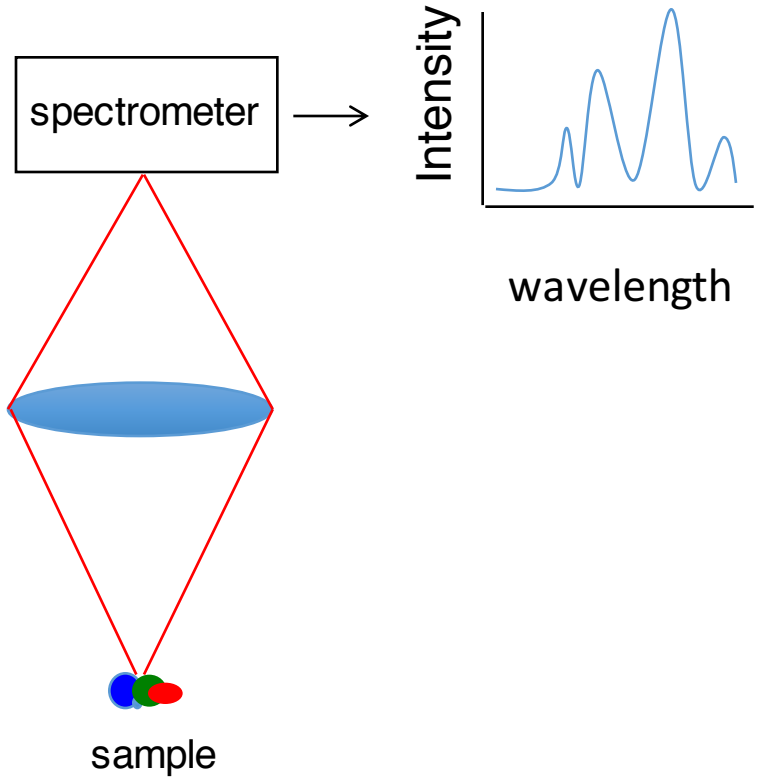
- Review spectral unmixing (last class)
- From optimization to machine learning
- Ingredients for ML
- Example: linear classification of images
  - Train/test data
  - Linear regression model
  - 3 ways to solve

Last time: simple example of spectral unmixing

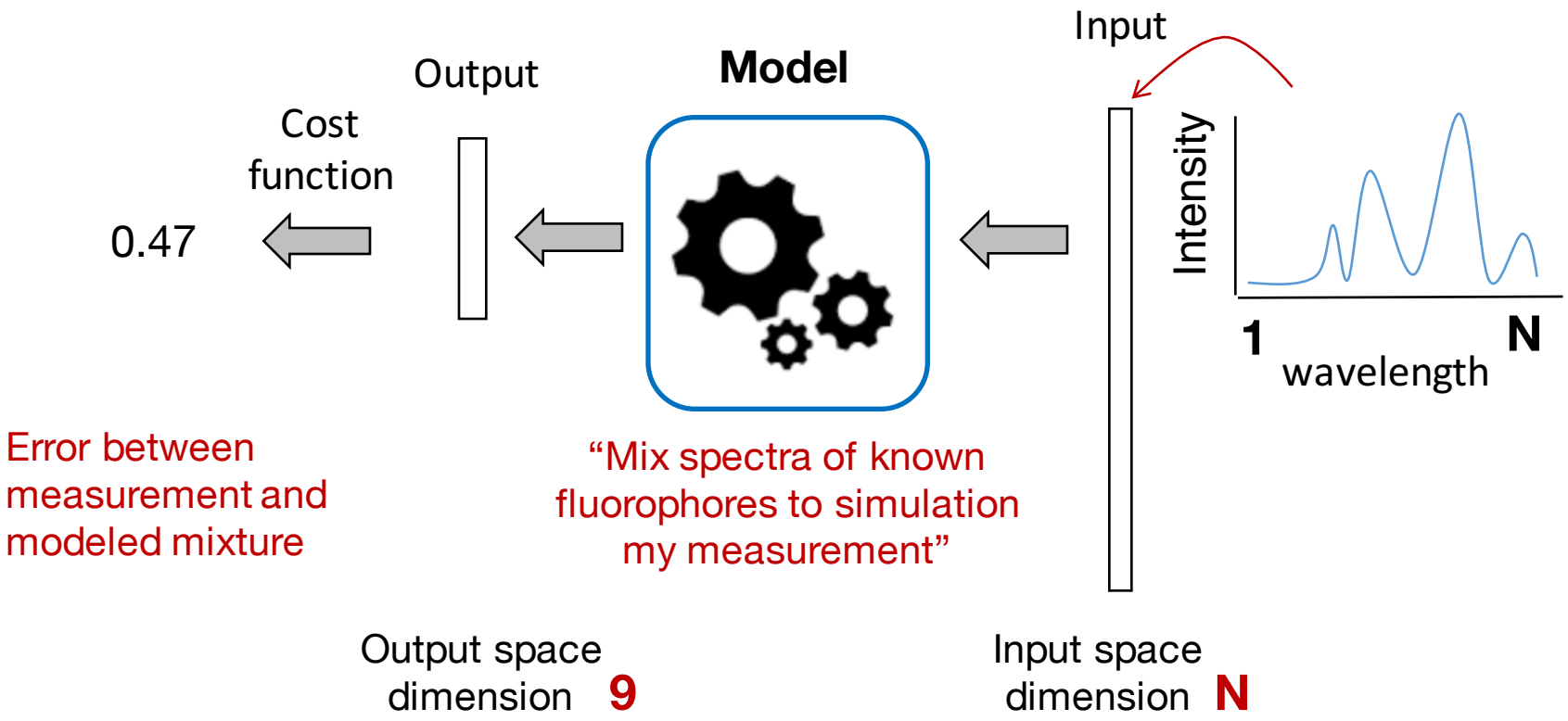
(For whatever reason, whenever I get confused about optimization, I think about this example)

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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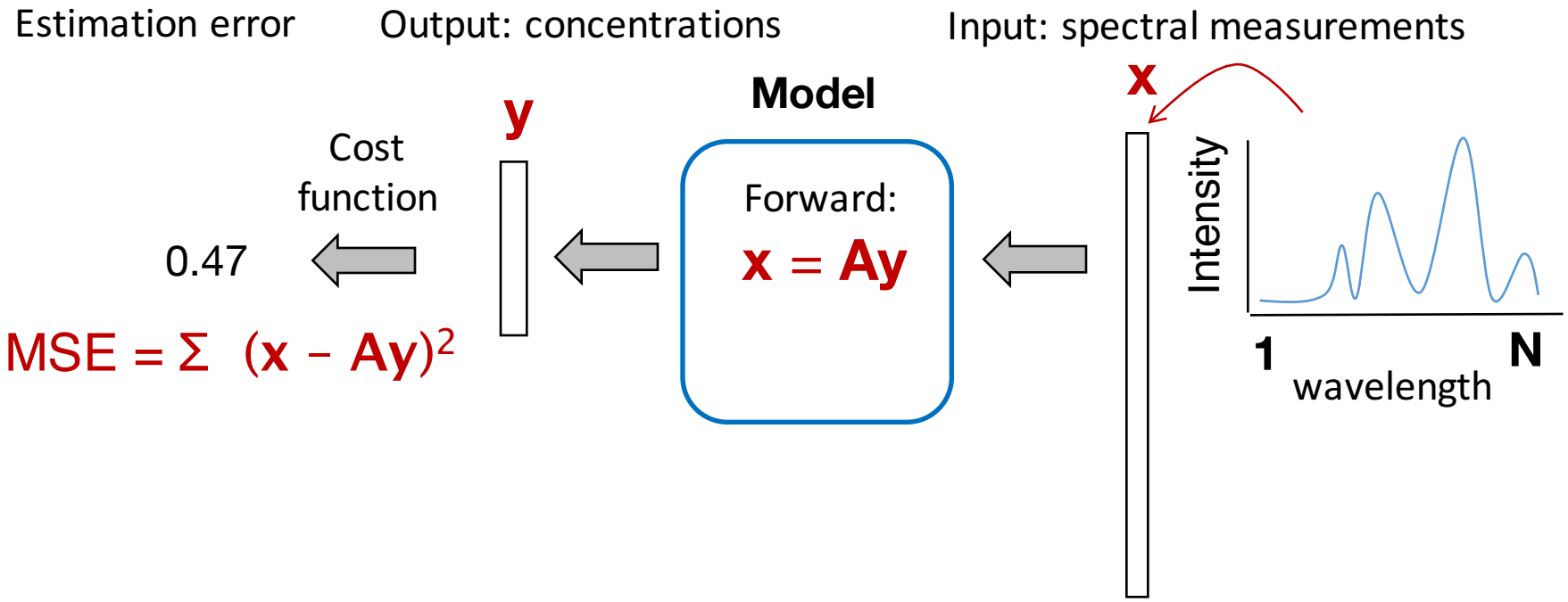
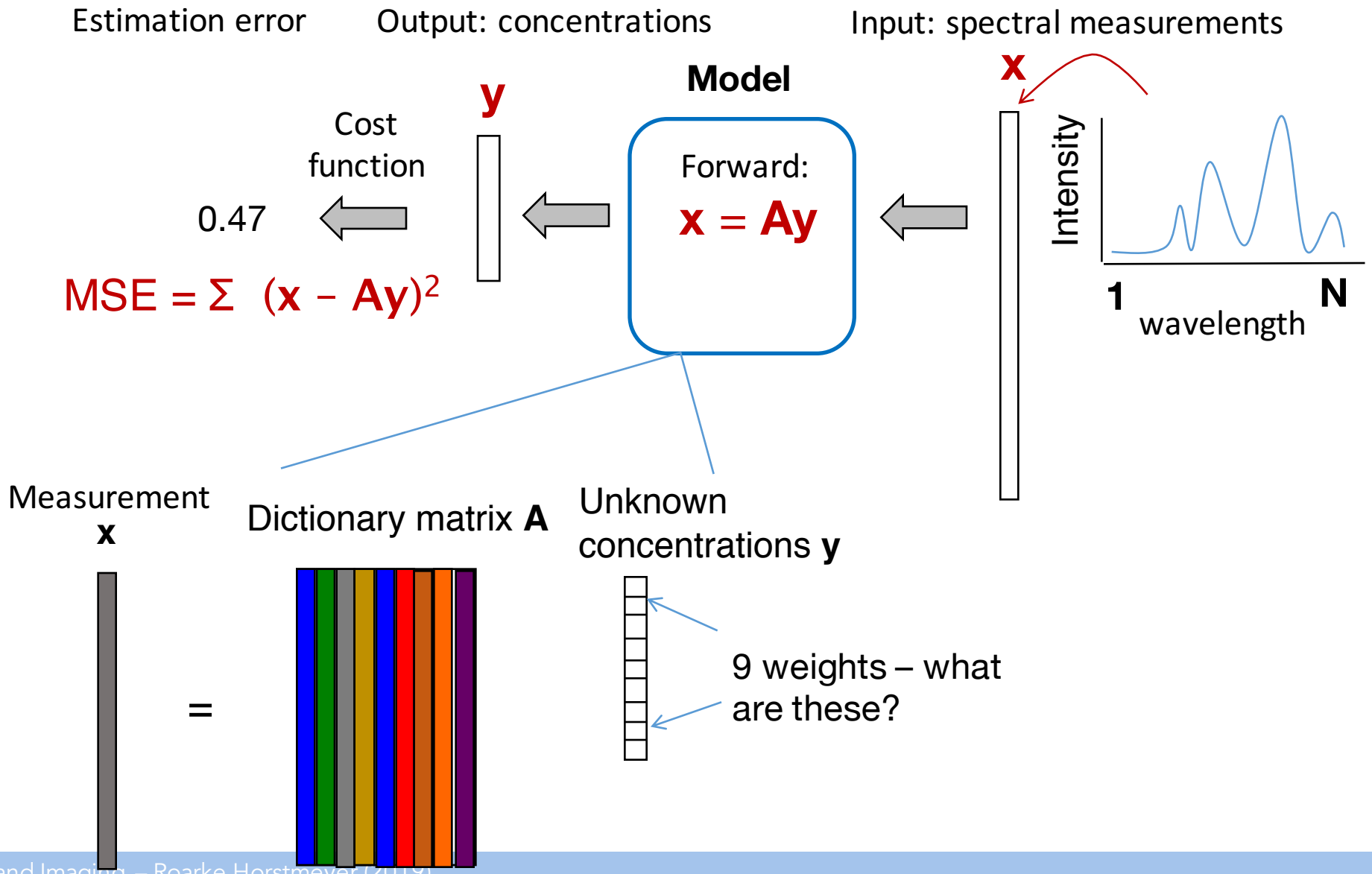


*Note: notation changed from last time to be consistent with we'll use in the future

Optimization pipeline for spectral unmixing



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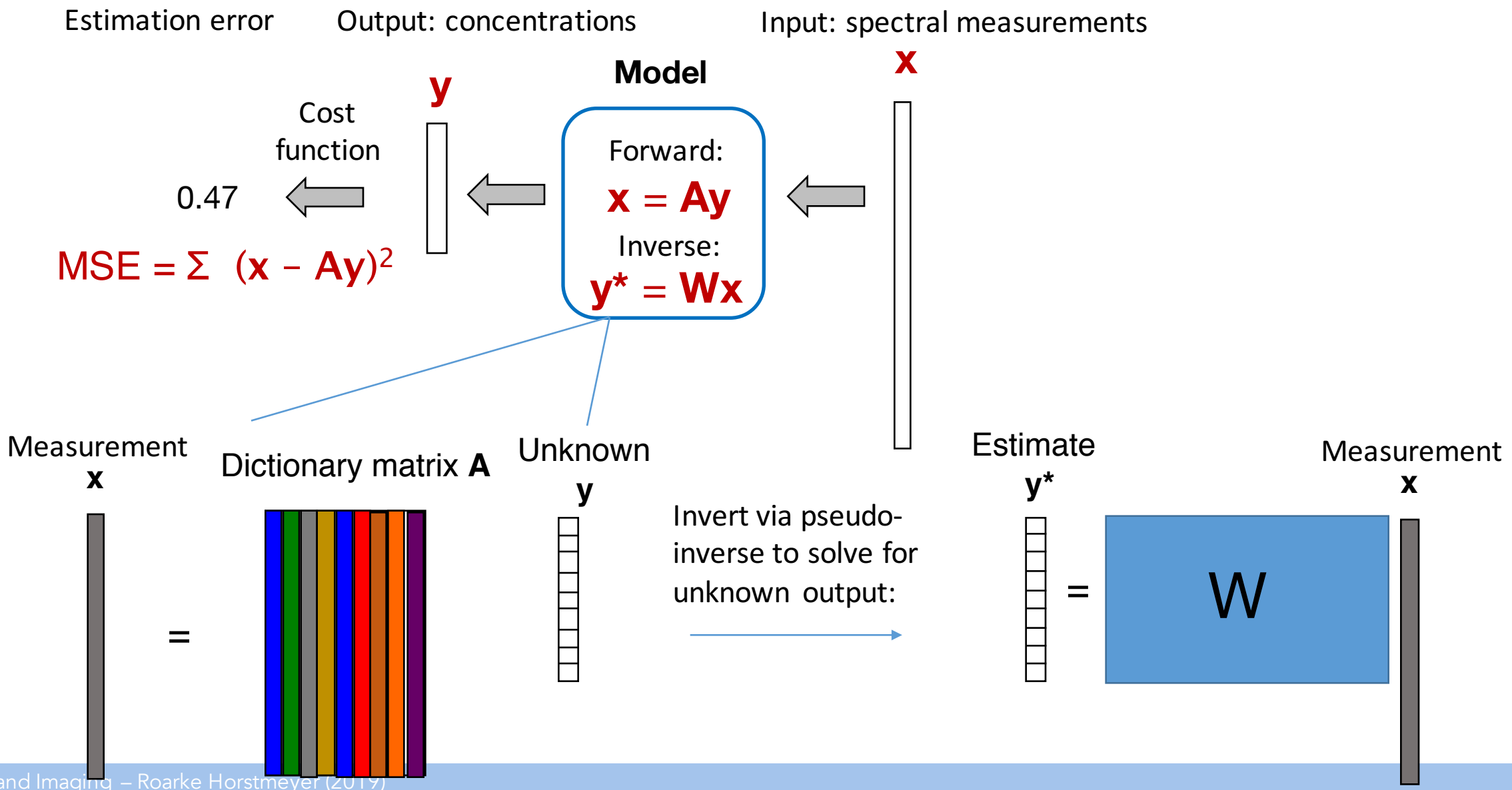

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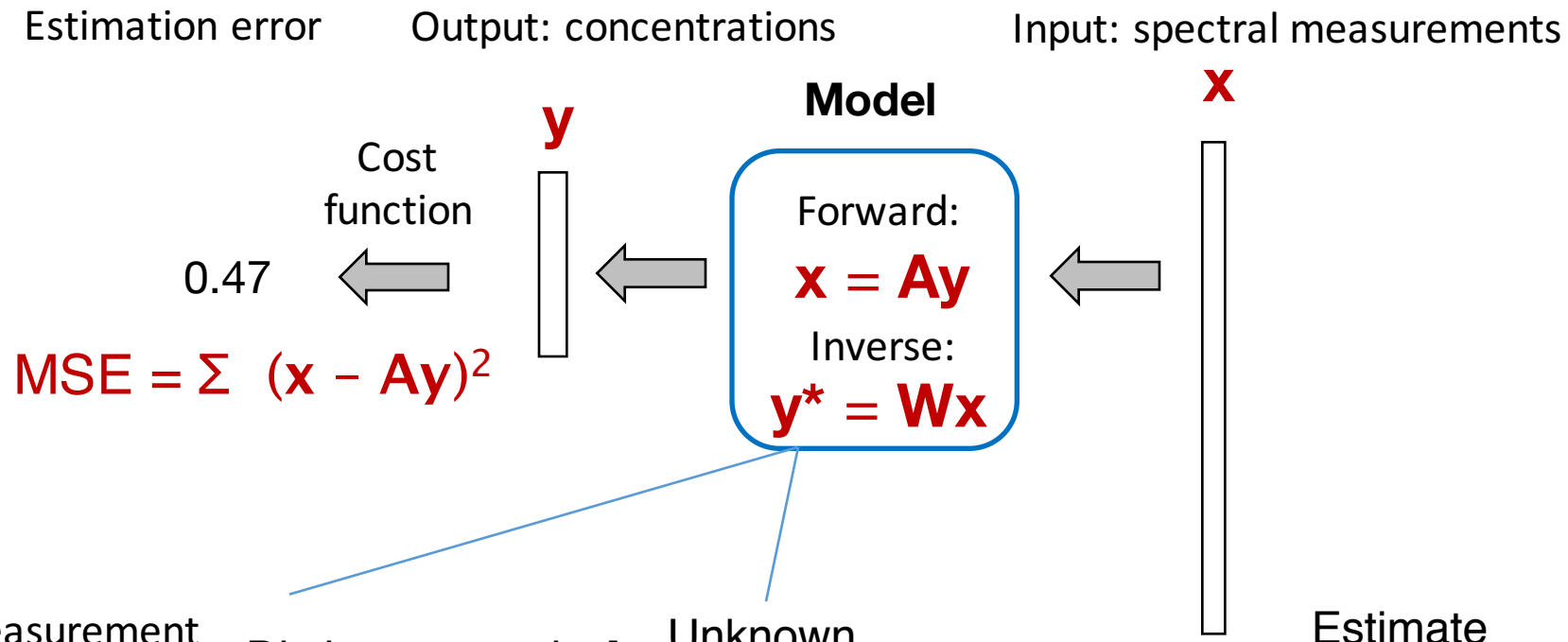
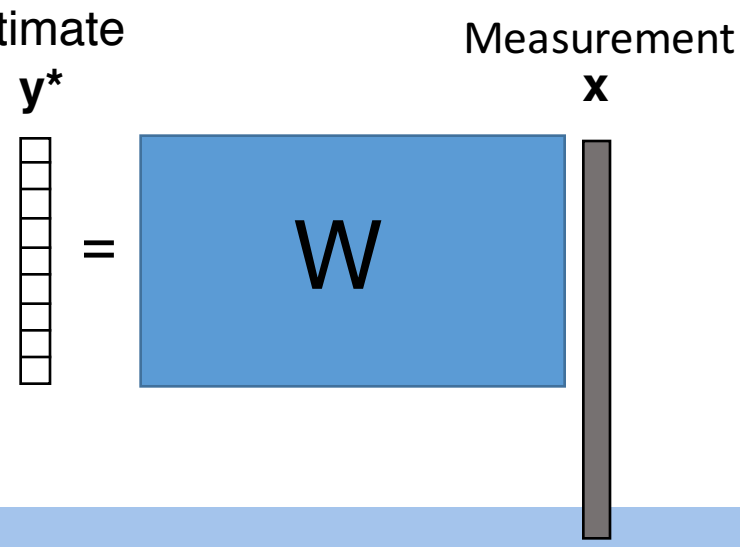


Invert via pseudo-inverse to solve for unknown output:

$$W = (A^T A)^{-1} A^T$$

$$y^* = Wx$$



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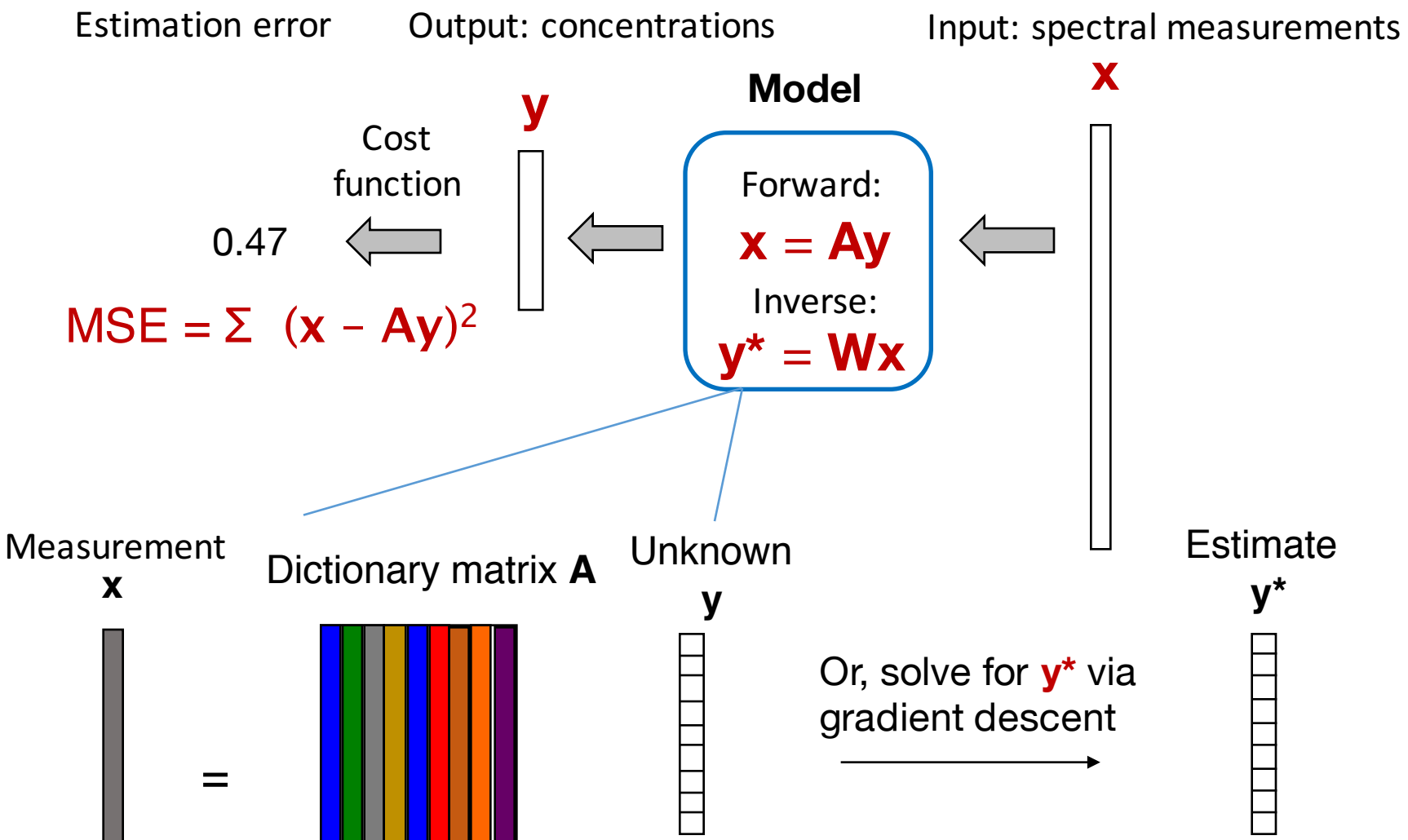
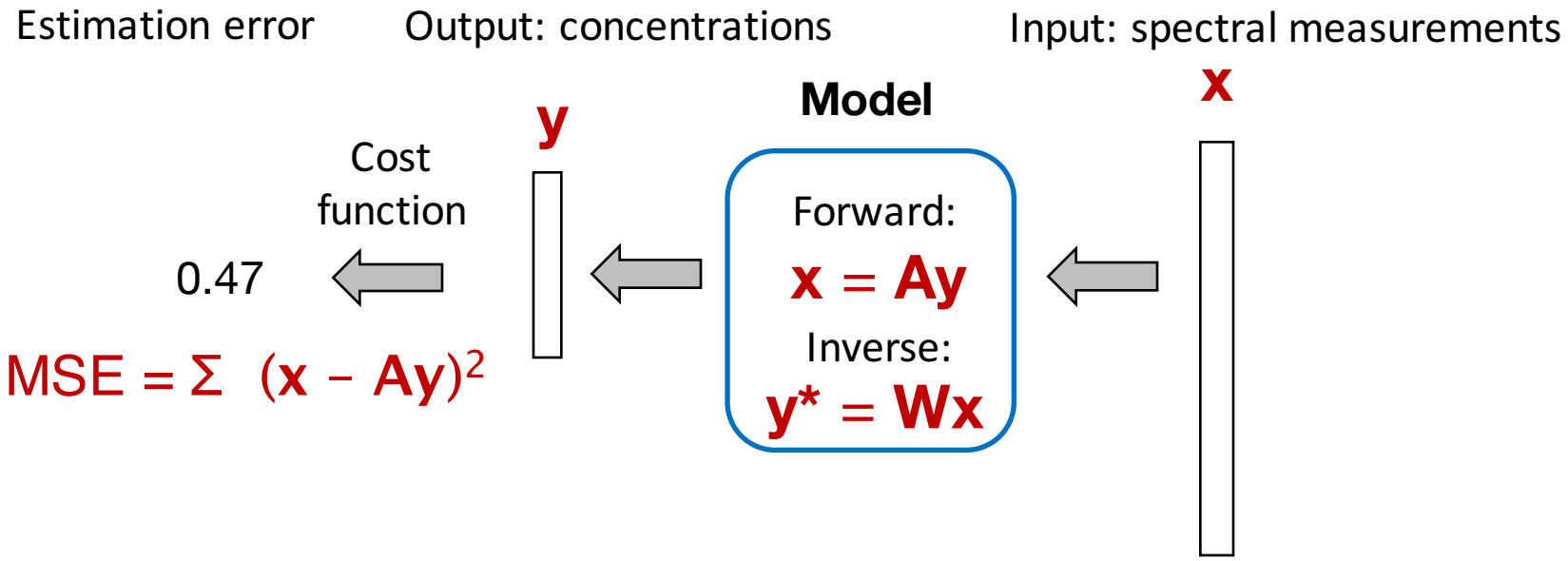
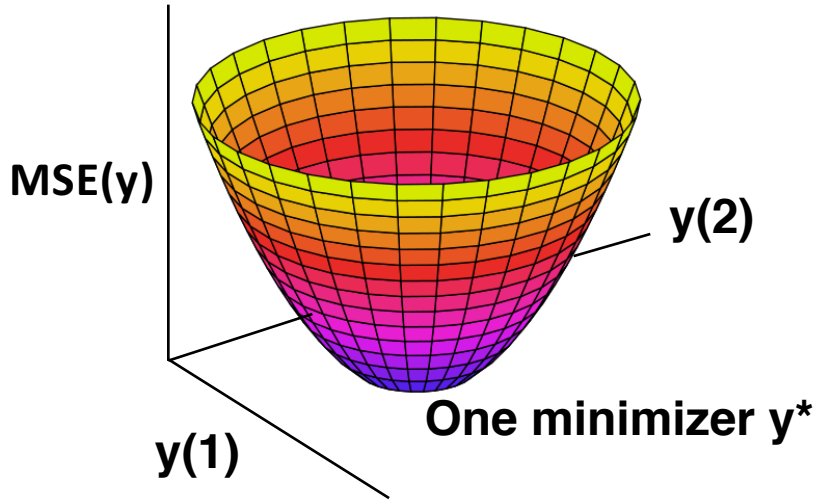


Optimization pipeline for spectral unmixing

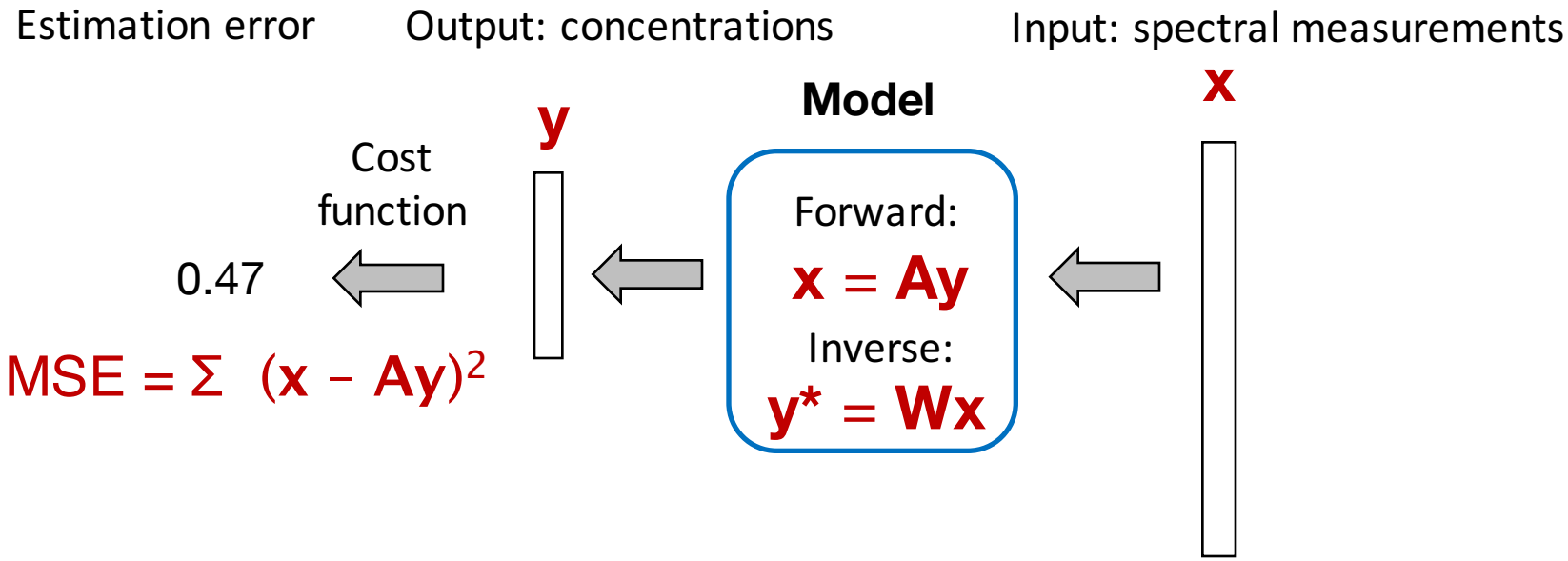


$$MSE(\mathbf{y}) = \sum_{\text{spectral measurements}} (\mathbf{x} - \mathbf{A}\mathbf{y})^2$$

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

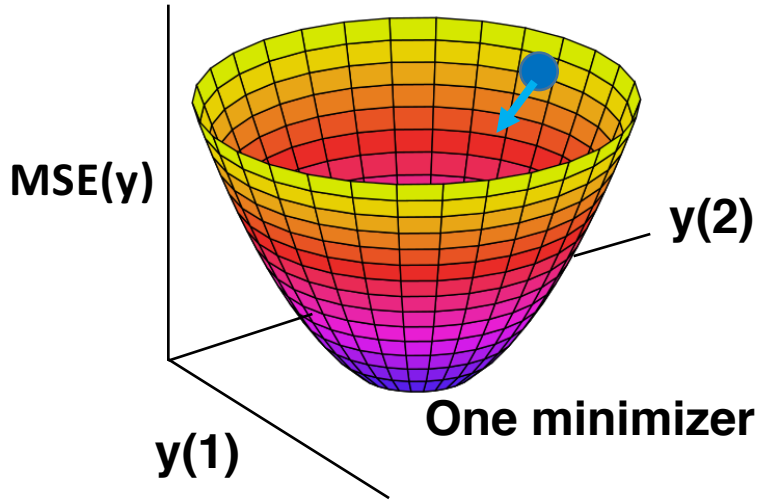


Optimization pipeline for spectral unmixing



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

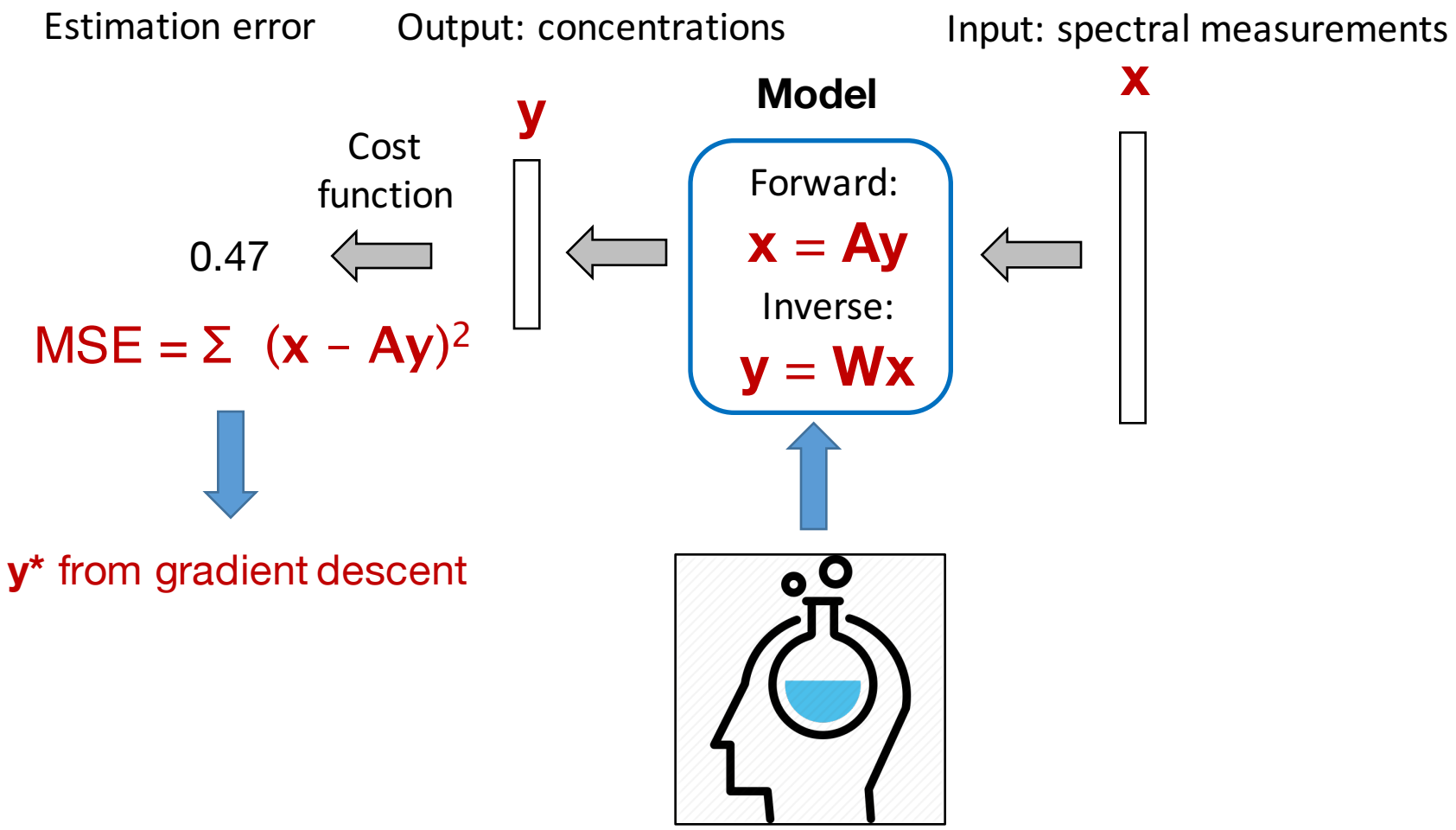
$$d/d\mathbf{y}\ MSE = \mathbf{A}^T(\mathbf{x} - \mathbf{Ay})$$



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

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

Optimization pipeline for spectral unmixing



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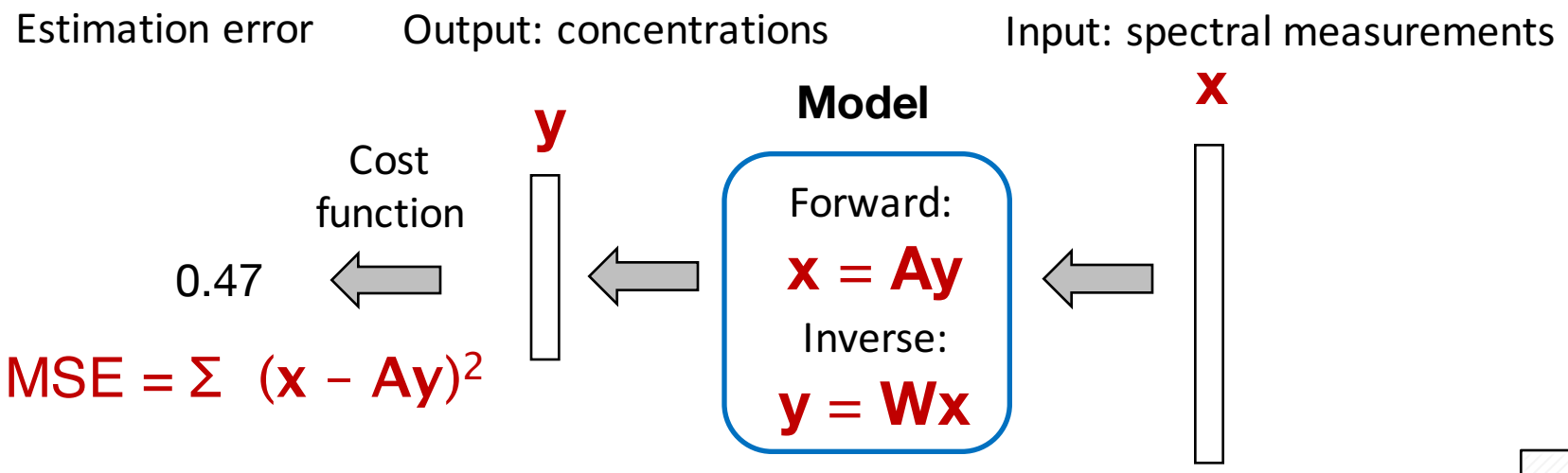
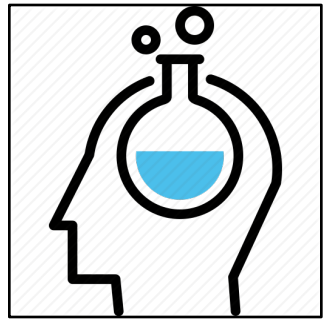
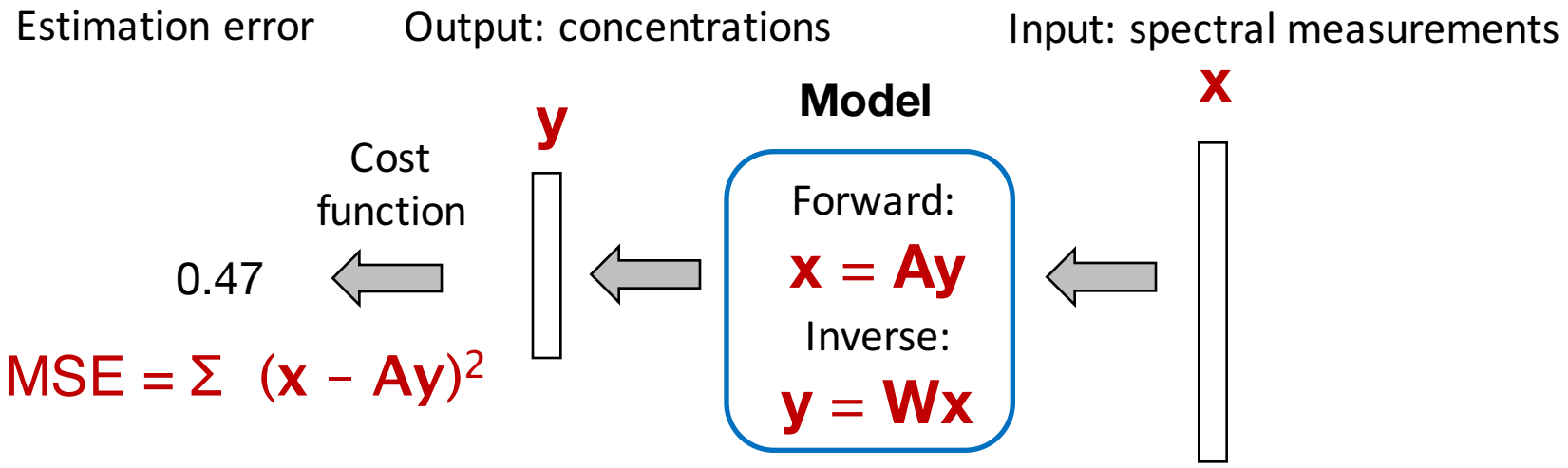




A and **W** from first principles

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

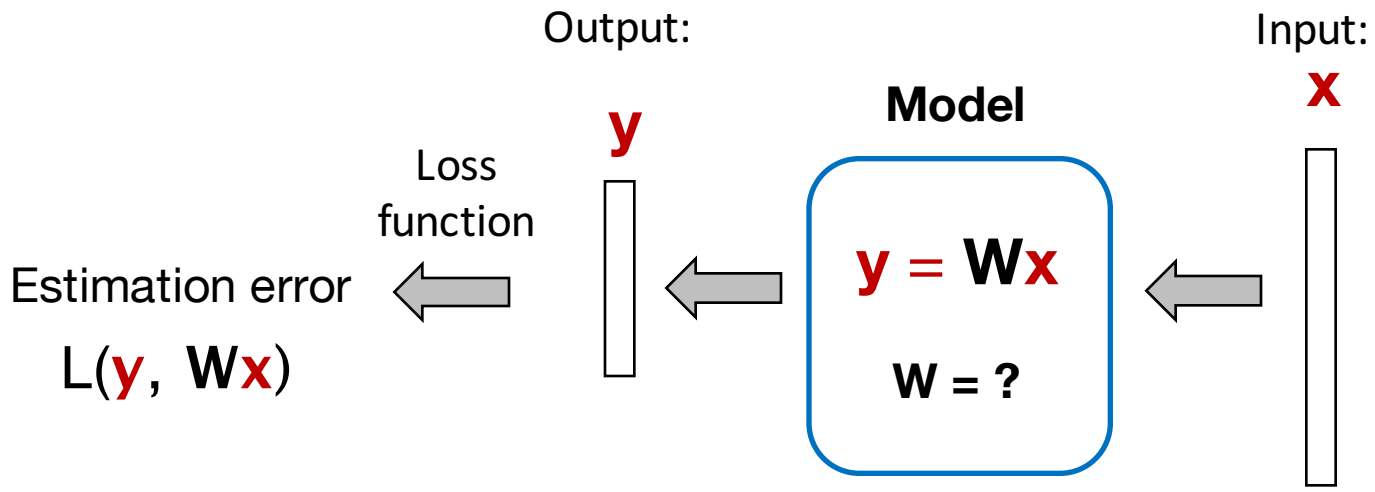
Optimization pipeline for spectral unmixing



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***

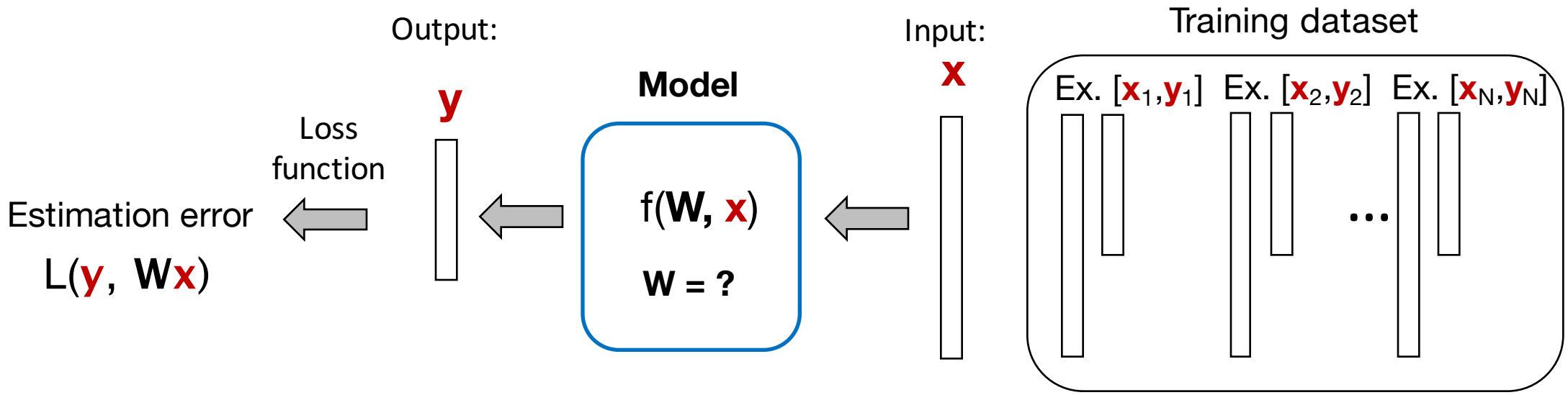
Pipeline for machine learning



Changes for machine learning framework:

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

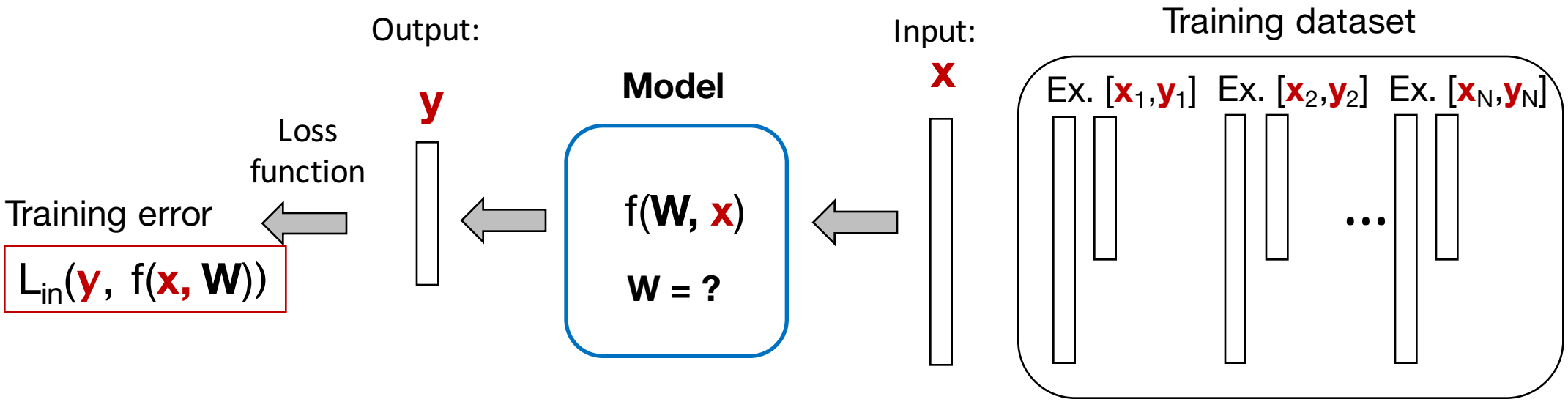
Pipeline for machine learning



Changes for machine learning framework:

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

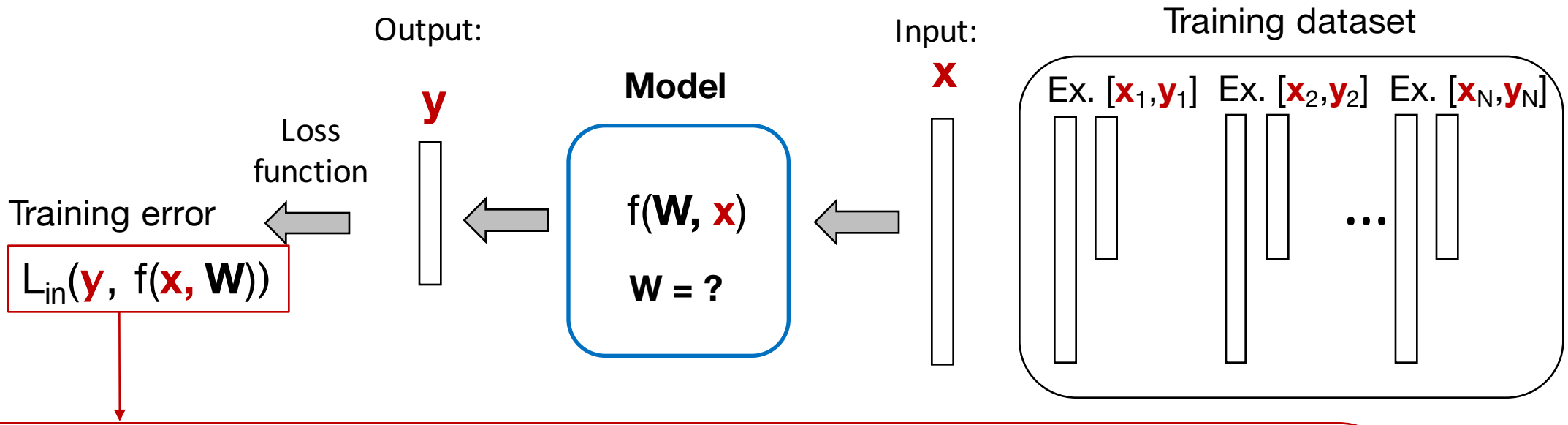
Pipeline for machine learning



Changes for machine learning framework:

1. Now must 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. To do so, use a *loss function* L that depends upon the training inputs (x,y) *and* the model (**W**)

Pipeline for machine learning

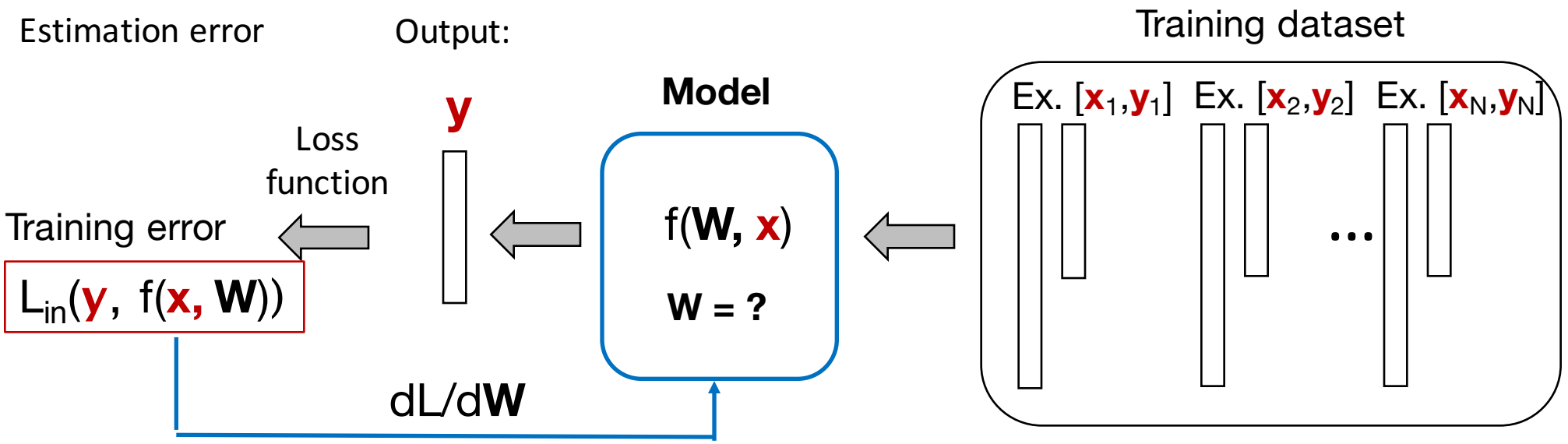


Training Error ("in class error"):

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

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

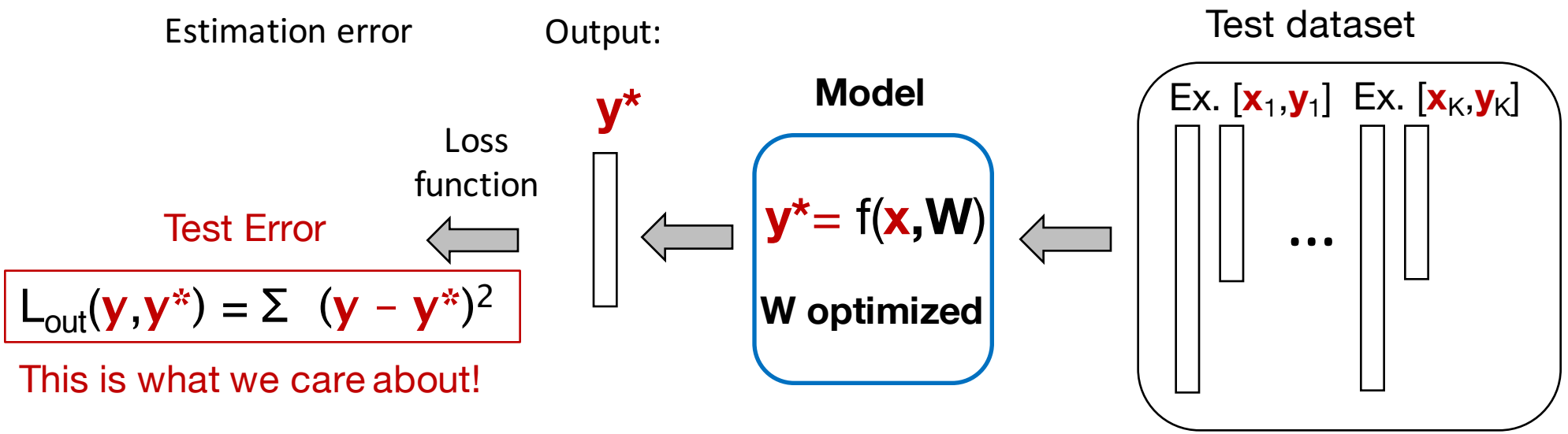
Pipeline for machine learning



Changes for machine learning framework:

1. Now must 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. To do so, use a *loss function* L that depends upon the training inputs (x,y) *and* the model (**W**)
4. Find optimal mapping (**W**) using the training data, guided by 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, guided by 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

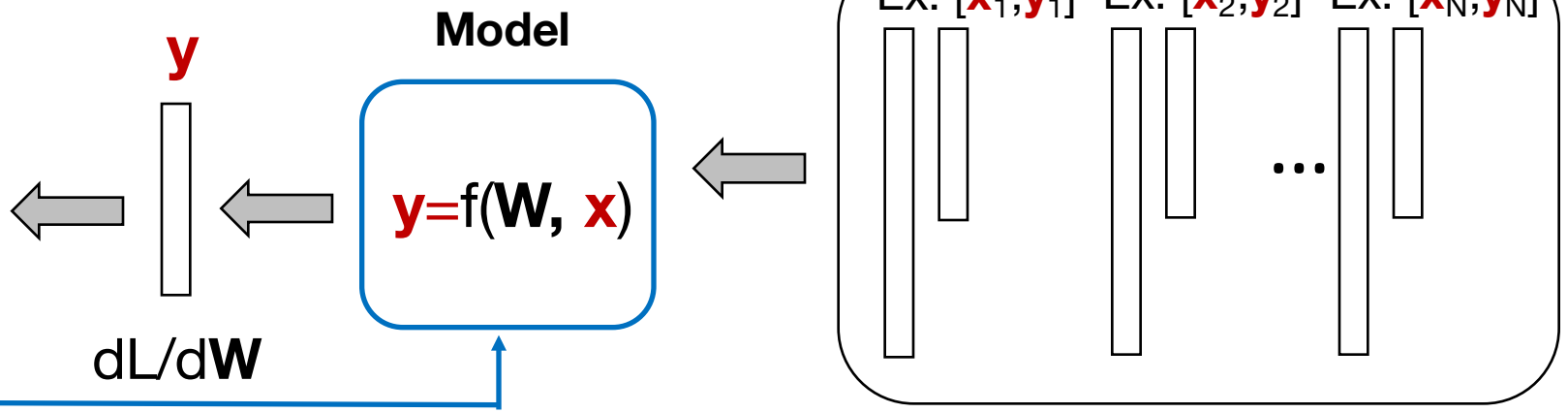
Correct labels for test images?

Output: Image class

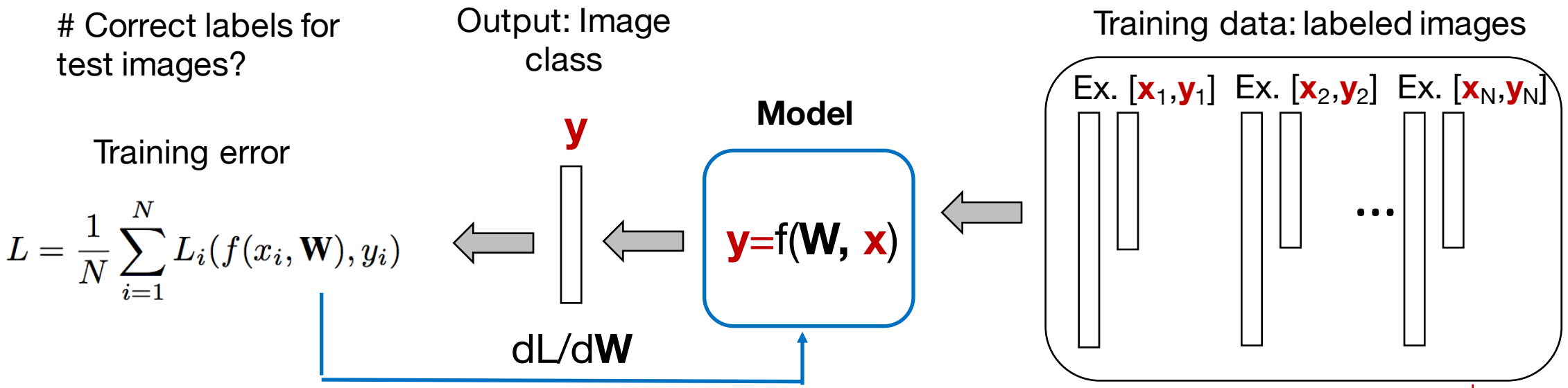
Training data: labeled images

Training error

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



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

https://en.wikipedia.org/wiki/MNIST_database

MNIST image set: http://yann.lecun.com/exdb/mnist/

Example: MNIST image dataset

M = 28x28 pixel matrix

m = vec[M] = 784-long vector

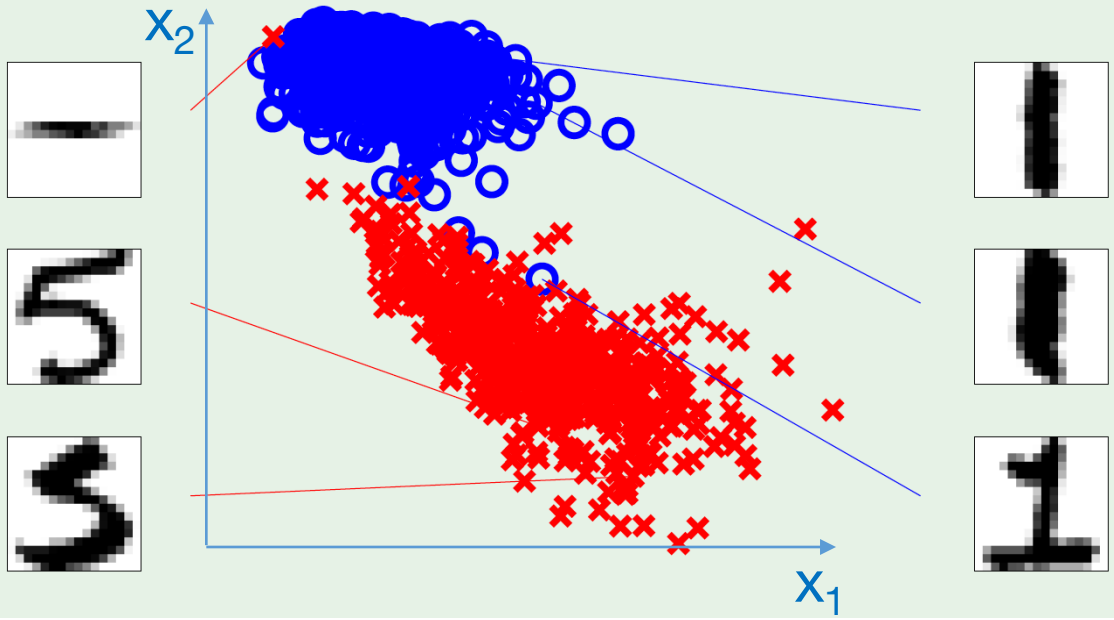
Linear model would require W = 784 element matrix

Start simple: use $x = (x_0, x_1, x_2)$ to describe **intensity** and **symmetry** of M

Linear model can now use smaller $w = (w_0, w_1, w_2)$

Illustration of features

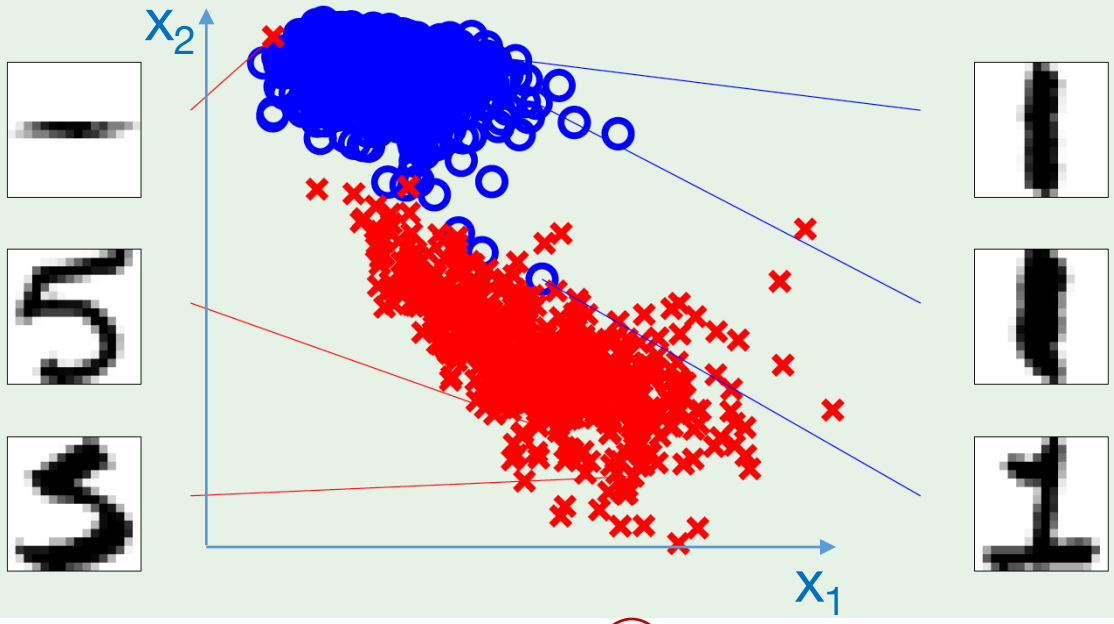
$\mathbf{x} = (x_0, x_1, x_2)$ x_1: intensity x_2: symmetry



Caltech Learning from Data: https://work.caltech.edu/telecourse.html

Illustration of features

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



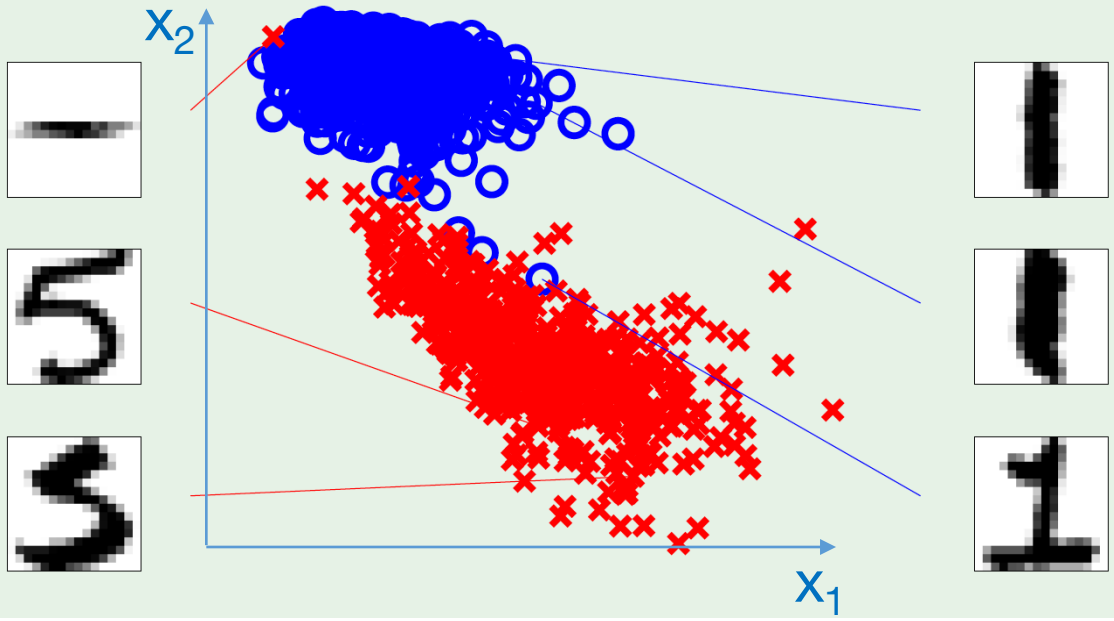
Dataset: 1000 examples of 1's and 5's mapped to $\mathbf{x}_j = (1, x_1, x_2)$, with associated label $y_j = 1$ or -1

This transforms wx+b into **wx**

Caltech Learning from Data: https://work.caltech.edu/telecourse.html

Illustration of features

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



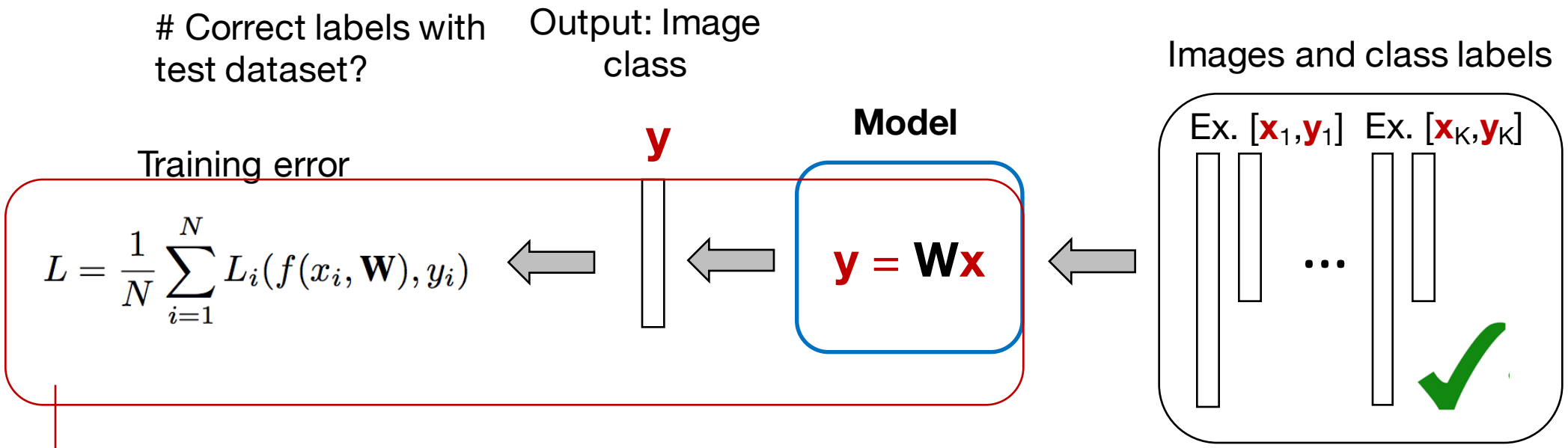
Dataset: 1000 examples of 1's and 5's mapped to $\mathbf{x}_j = (1, x_1, x_2)$, with associated label $y_j = 1$ or -1

$[\mathbf{X}_{train}, \mathbf{Y}_{train}] = [\mathbf{x}_j, \mathbf{y}_j]$ 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

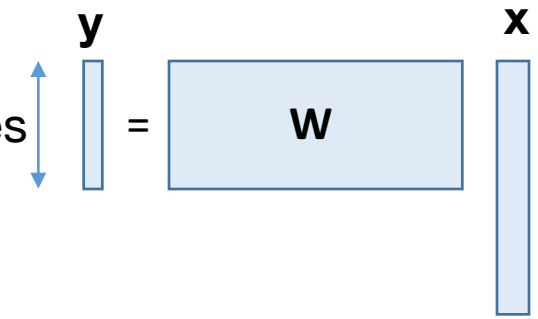
Let's start with a simpler approach: linear regression

deep imaging

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

General linear model:

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



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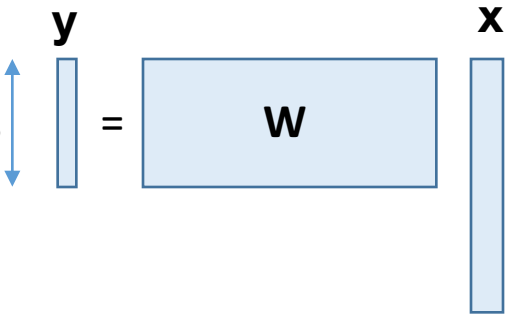
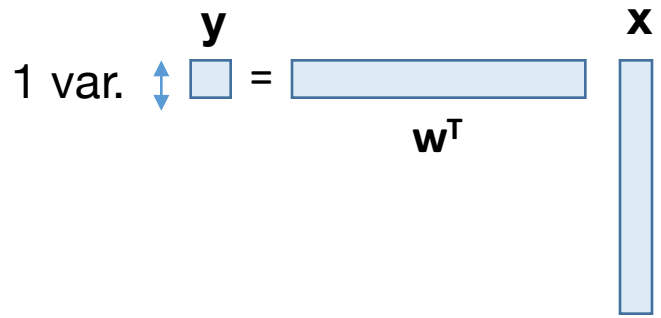


Assume 1 class = 1 linear fit

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



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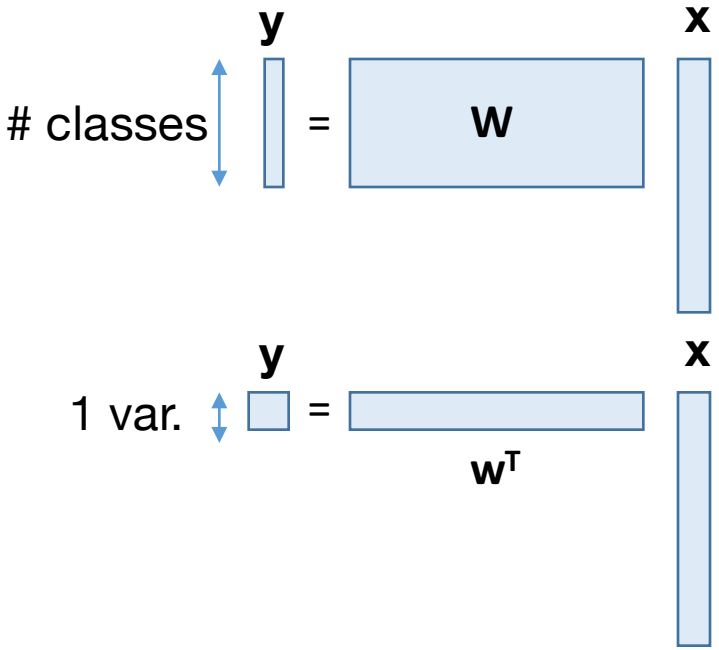


Assume 1 class = 1 linear fit

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

Use MSE error model

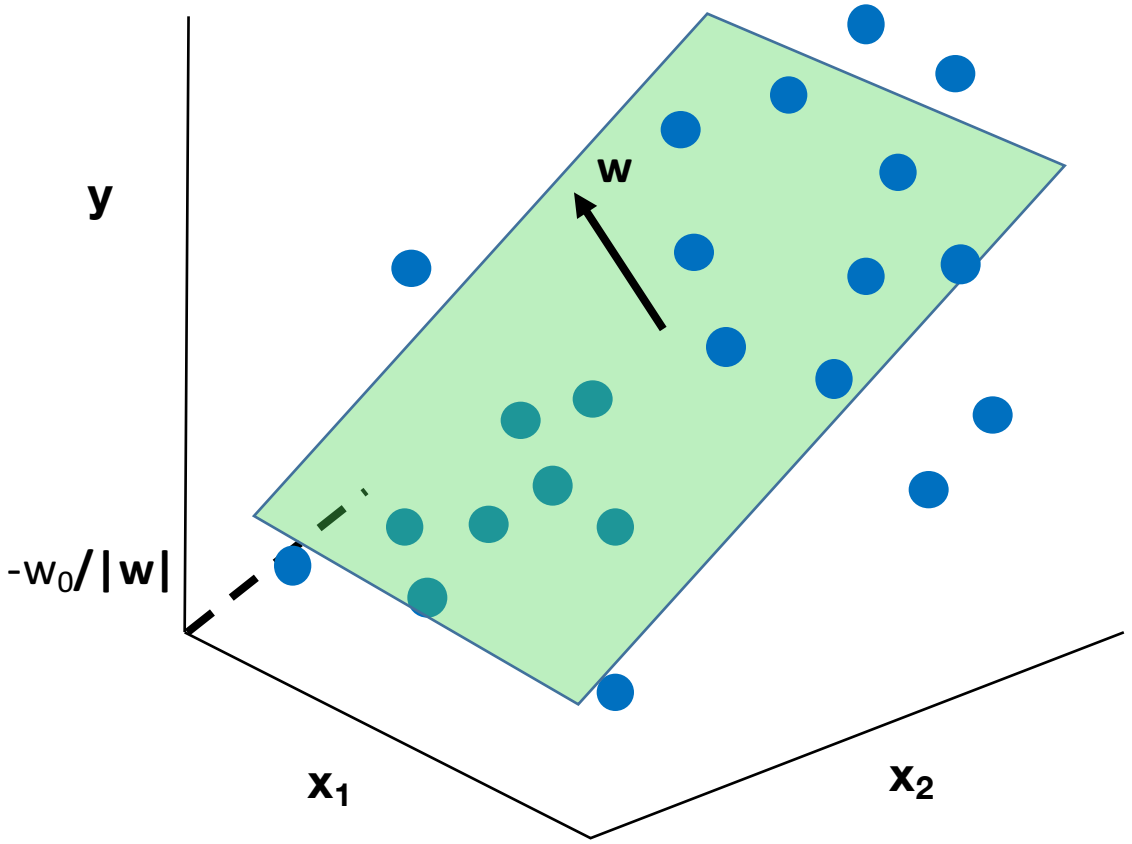
$$L = \frac{1}{N}\sum_{i=1}^{N} (w^T x_i - y_i)^2$$

Where labels determined by thresholding

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

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

Why does linear regression with sgn() achieve classification?



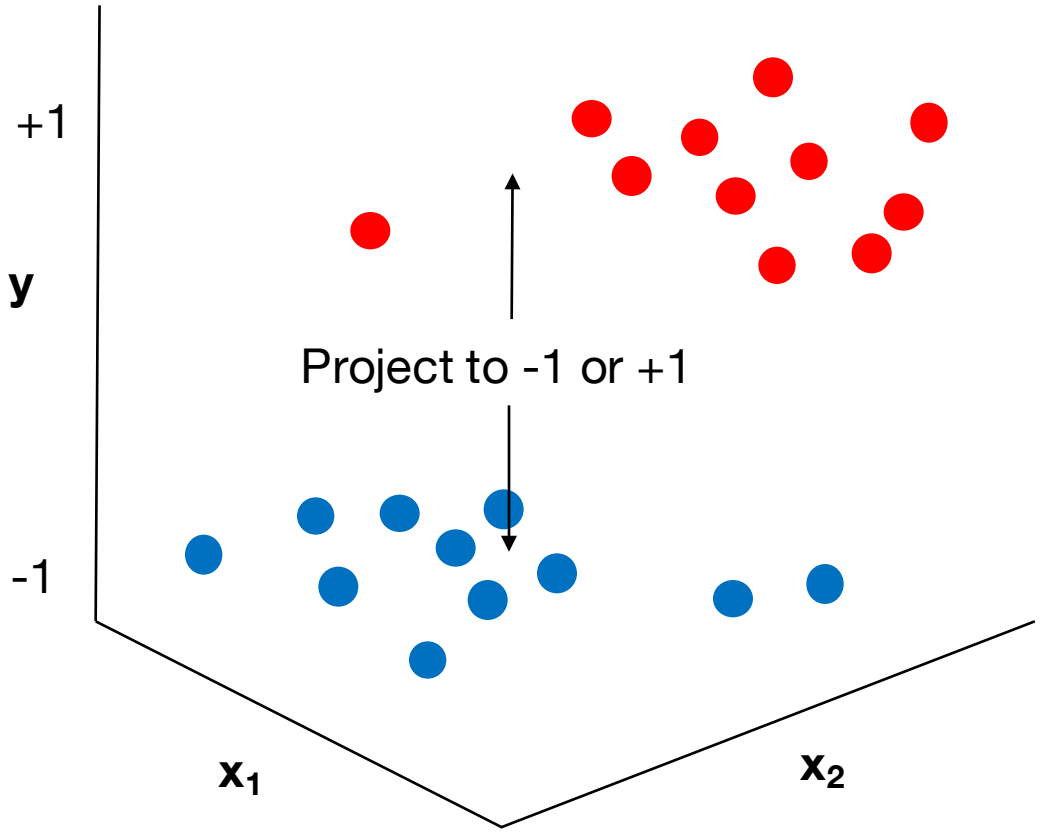
Without sgn(): regression for best fit

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

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

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

Why does linear regression with sgn() achieve classification?



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- y_i can only be -1 or +1, which defines its class

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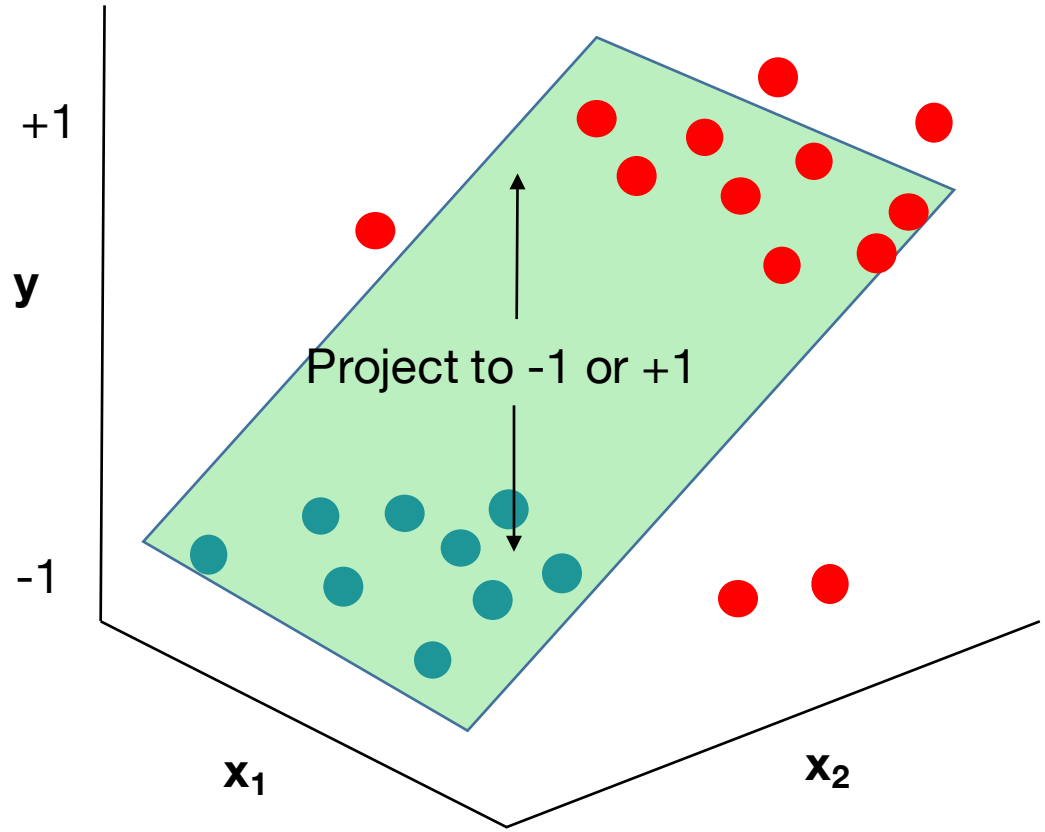

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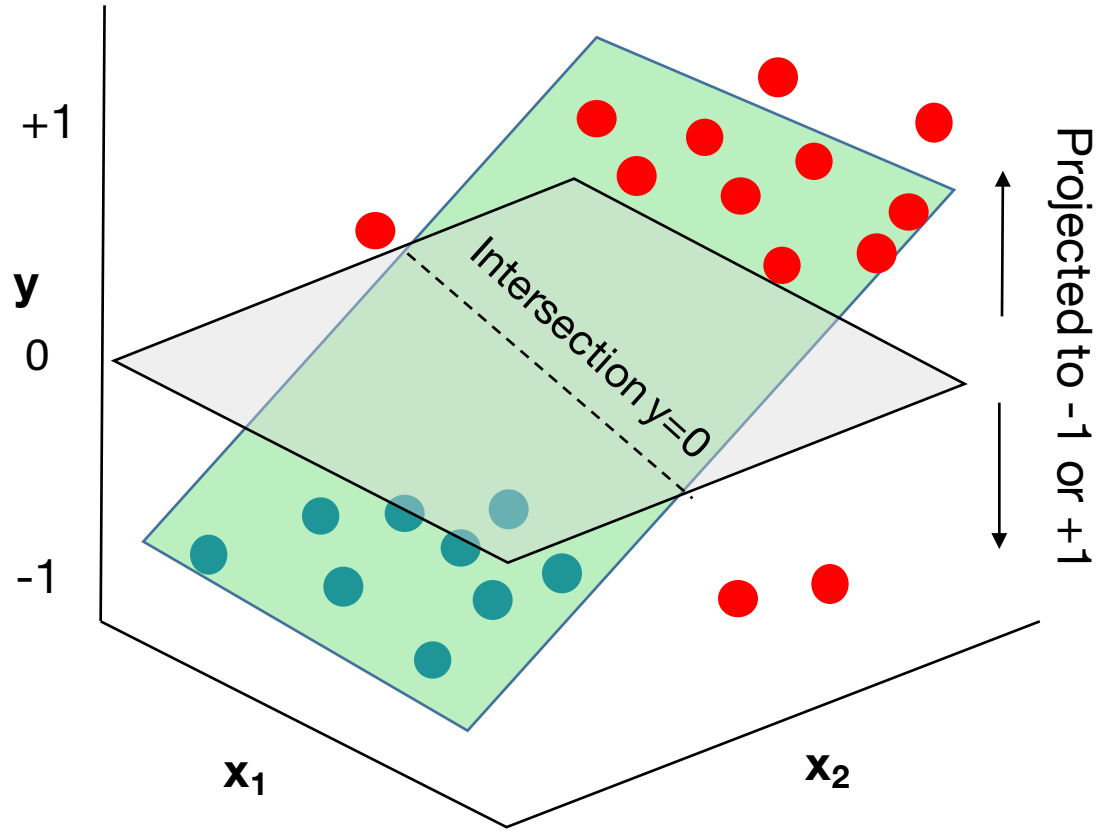
$$L = \frac{1}{N} \sum_{i=1}^{N} (w^T x_i - y_i)^2$$

- 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

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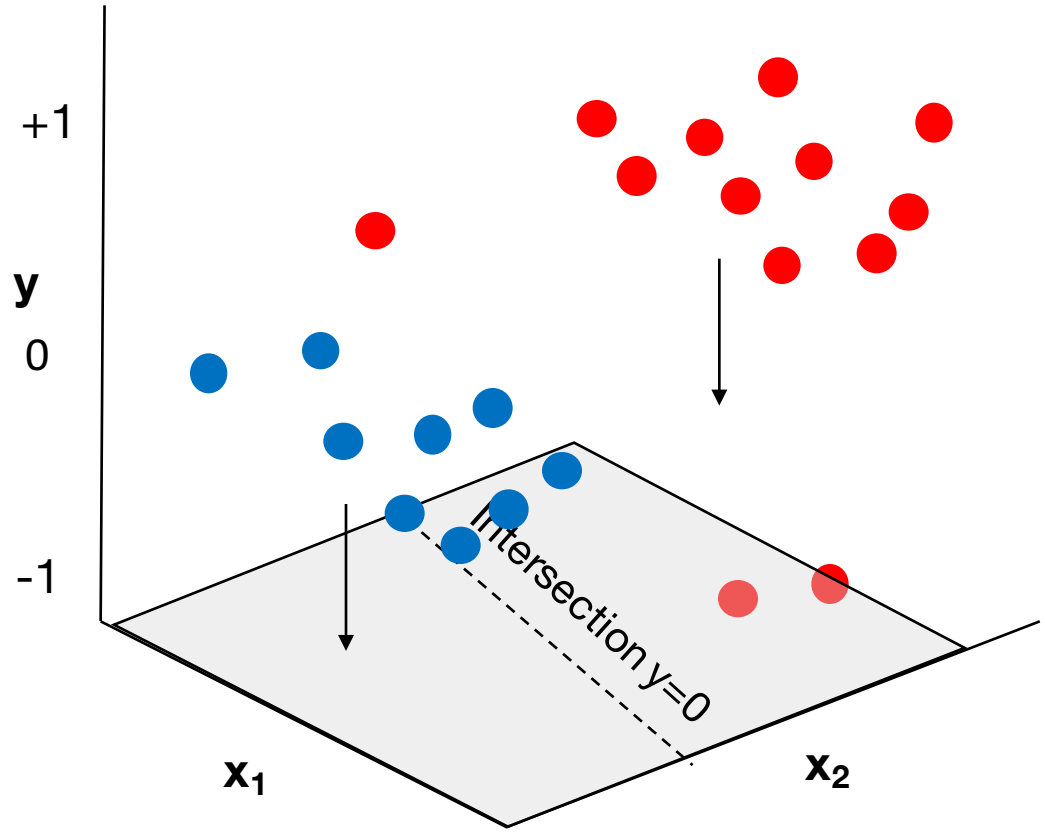

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- y axis isn't really needed now & can view this decision boundary in 2D

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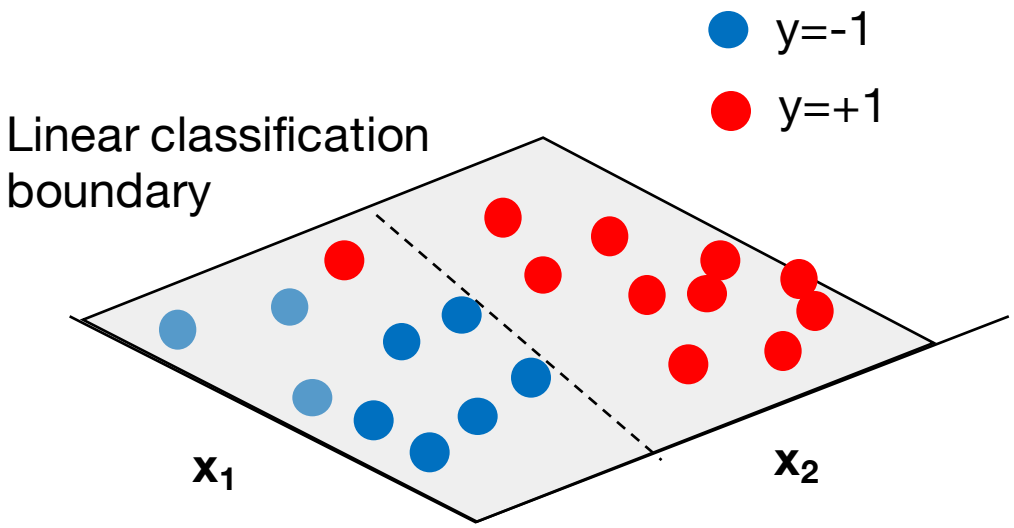
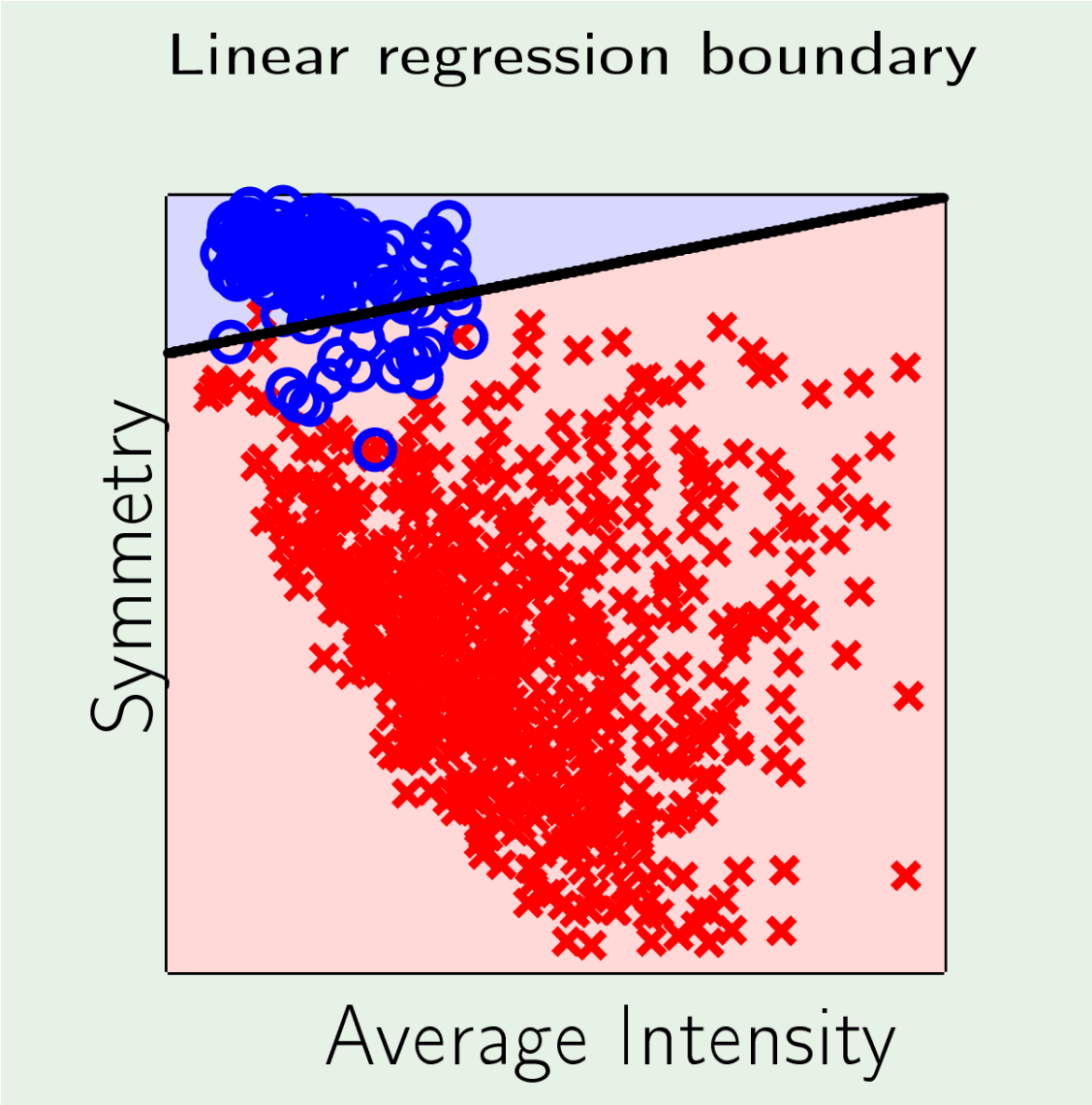
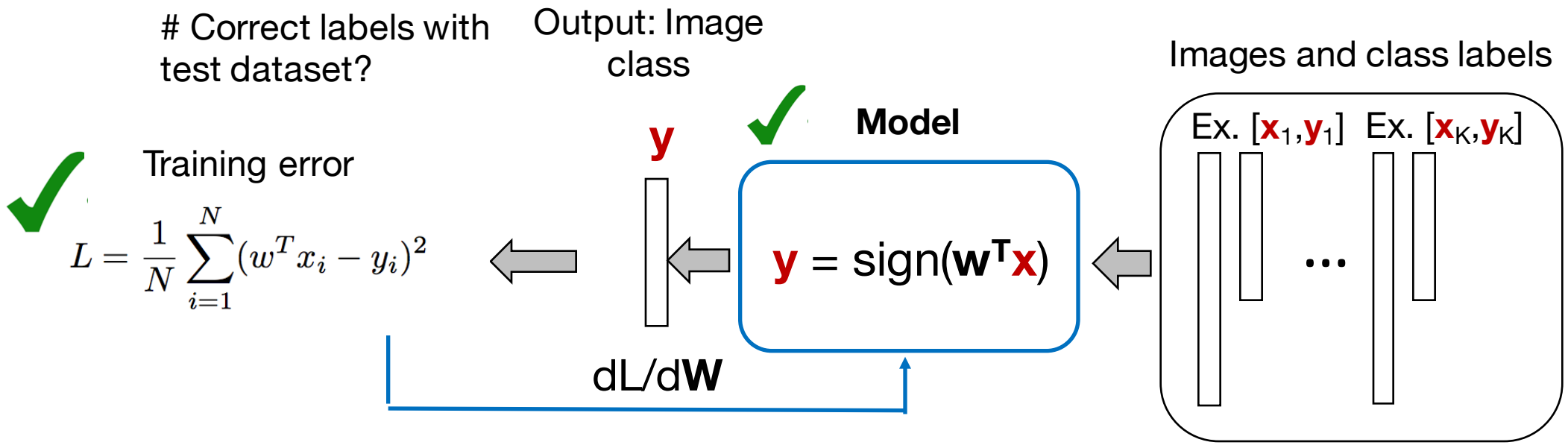


Sign operation takes linear regression and makes it a classification operation!



Caltech Learning from Data: https://work.caltech.edu/telecourse.html

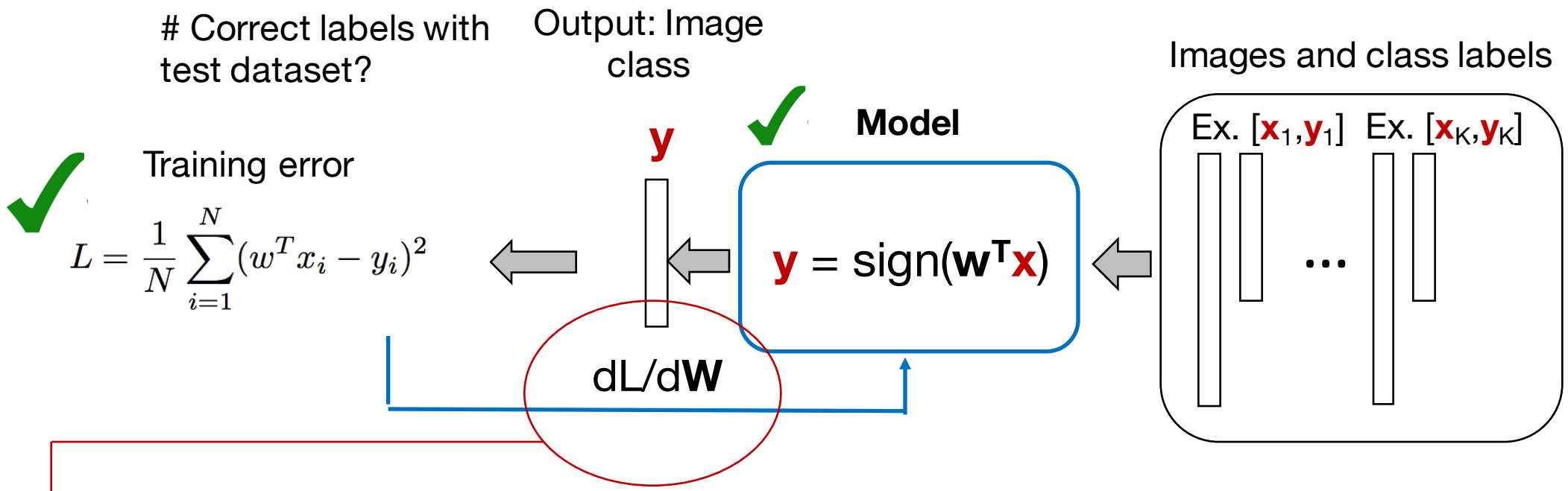
Example: machine learning for image classification



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**

Example: machine learning for image classification



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

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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)

1. Turning linear regression for unknown weights W in to a pseudo-inverse:

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

We are multiplying many x_i's with the same w and are adding them up - let's make a matrix!

$$X = \begin{vmatrix} x_1 \\ x_2 \\ \\ x_N \end{vmatrix}$$

Each training image is 1 row of X

$$y = \begin{vmatrix} y_1 \\ \\ \\ y_N \end{vmatrix}$$

Each training label is 1 entry of y

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

This is the same form as the pseudo-inverse we were working with before, but now we want to solve for *w*

Write this out as a matrix equation:

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

Note: Training data goes into “dictionary” matrix

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

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Take derivative wrt w and set to 0:

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

Solution is pseudo-inverse:

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

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Steps for Pseudo-inverse:

1. Construct matrix X and vector y from data

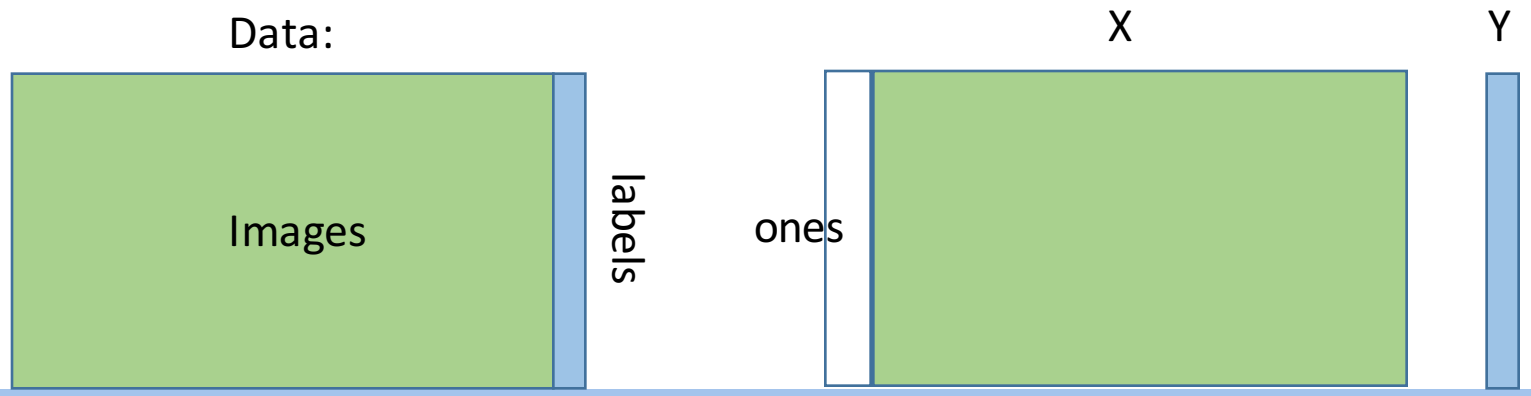
   Each training image is 1 row of X

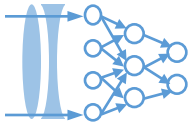
   Each training label is 1 entry of y

2. Compute solution for w_0 via above equation

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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(harder)

Gradient descent: The iterative recipe

deep imaging

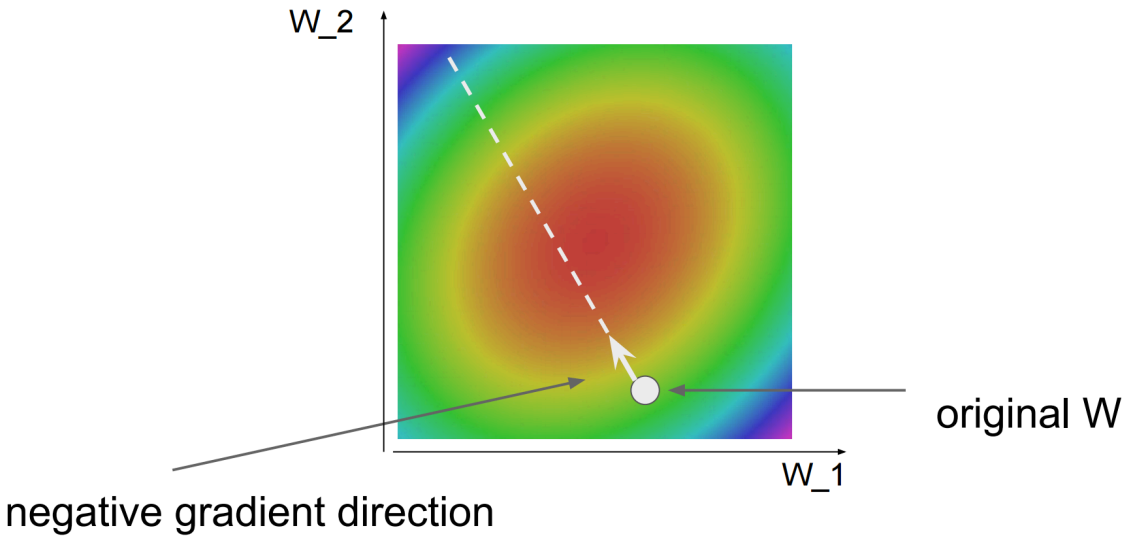
Initialize: Start with a guess of **W**

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:

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

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Example:

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

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Example:

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L(W, x, y) = 12.79

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

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

d$L(W_1)$/dW_1 = 10

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

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Next class: We'll go over how gradient descent works, and then examine the cost function to see why it really matters and how we can extend things beyond the simple case of linear regression