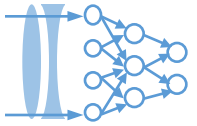
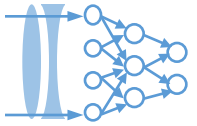


Machine Learning in Imaging

BME 590L
Roarke Horstmeyer

Lecture 7: Gradient descent and going beyond linear classification

Summary of machine learning pipeline:



1. Network Training

What we need for network training:

1. Labeled examples

Summary of machine learning pipeline:

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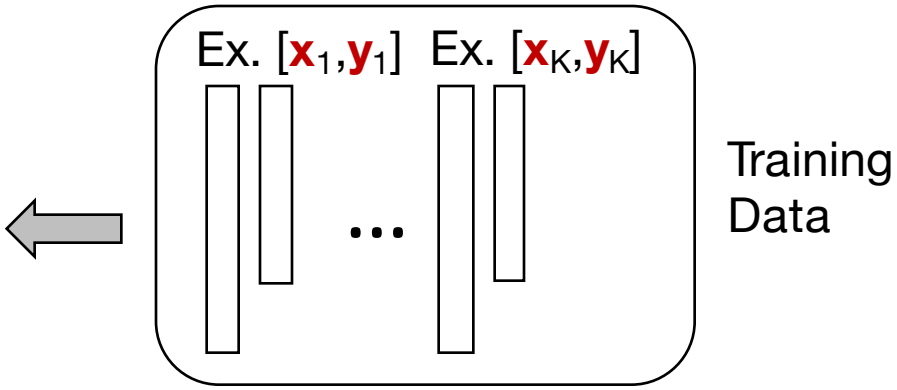
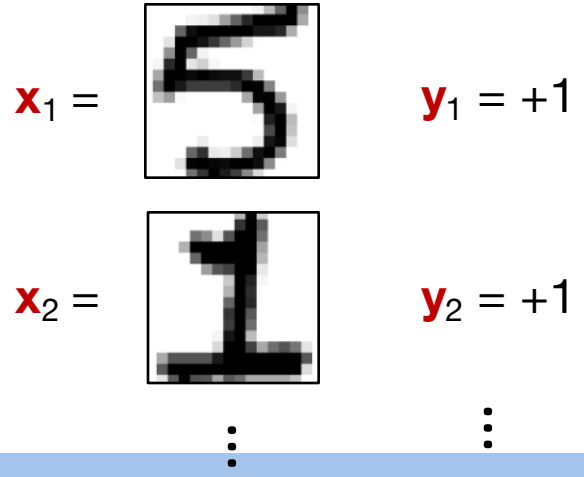


What we need for network training:

1. Labeled examples

E.g., images of 1's and 5's with labels:



Summary of machine learning pipeline:

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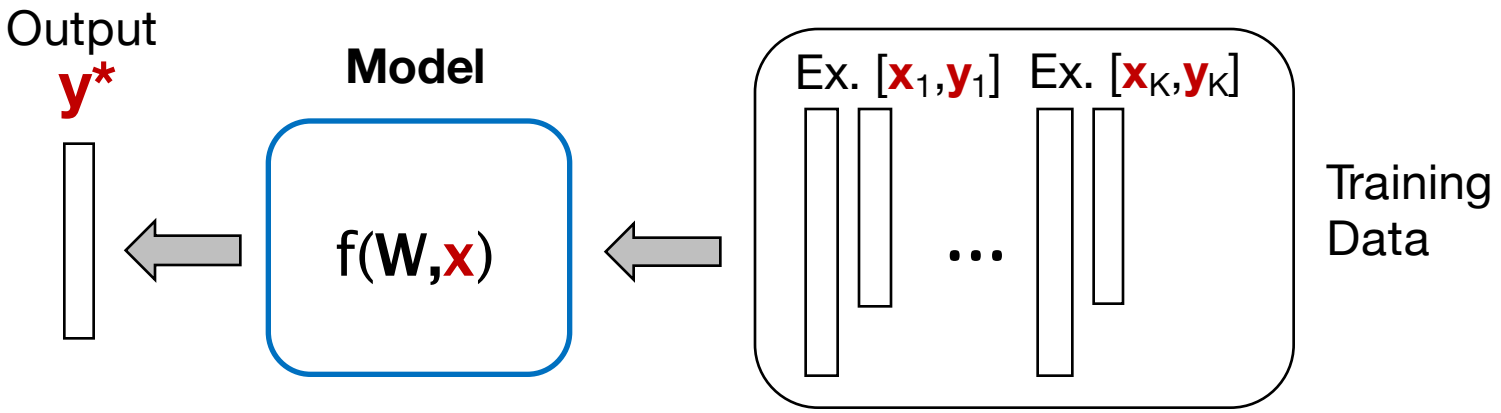

What we need for network training:

1. **Labeled examples**
2. **A model and loss function**

Summary of machine learning pipeline:

deep imaging

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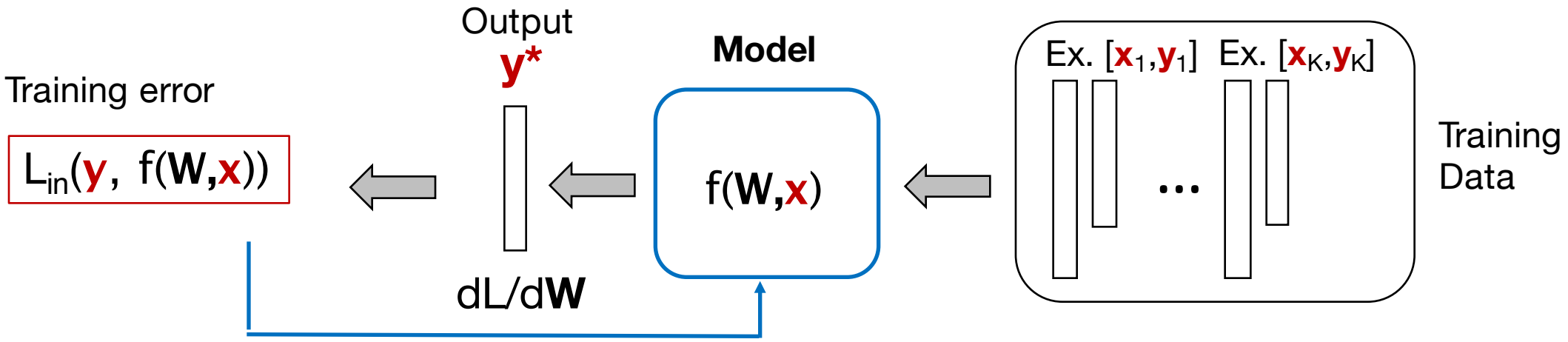
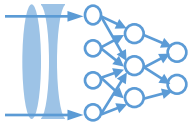


What we need for network training:

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

Summary of machine learning pipeline:

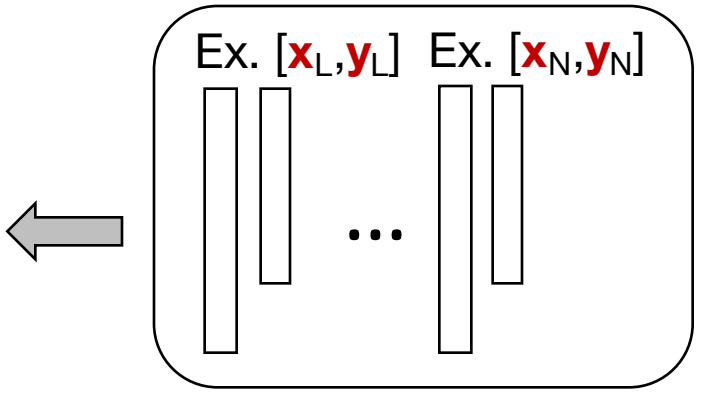


2. Network Testing

What we need for network testing:

Summary of machine learning pipeline:

2. Network Testing



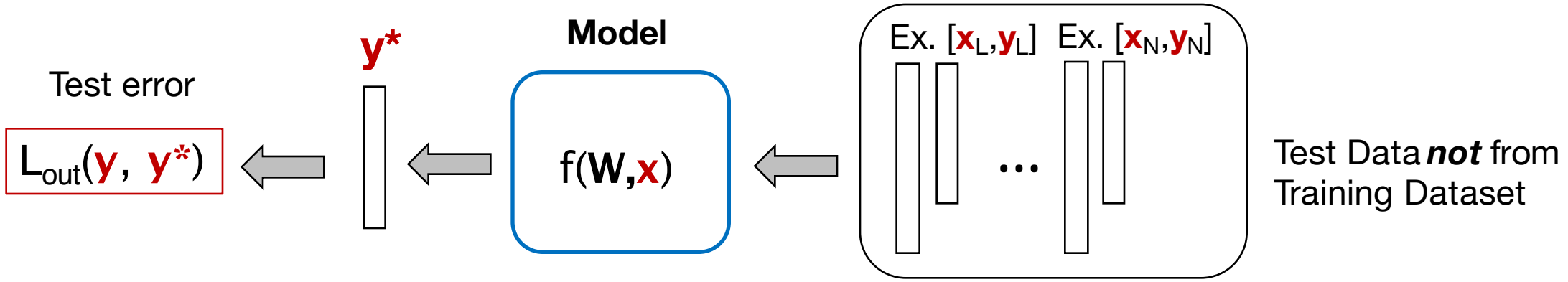
Test Data ***not*** from Training Dataset

What we need for network testing:

4. *Unique* labeled test data

Summary of machine learning pipeline:

2. Network Testing

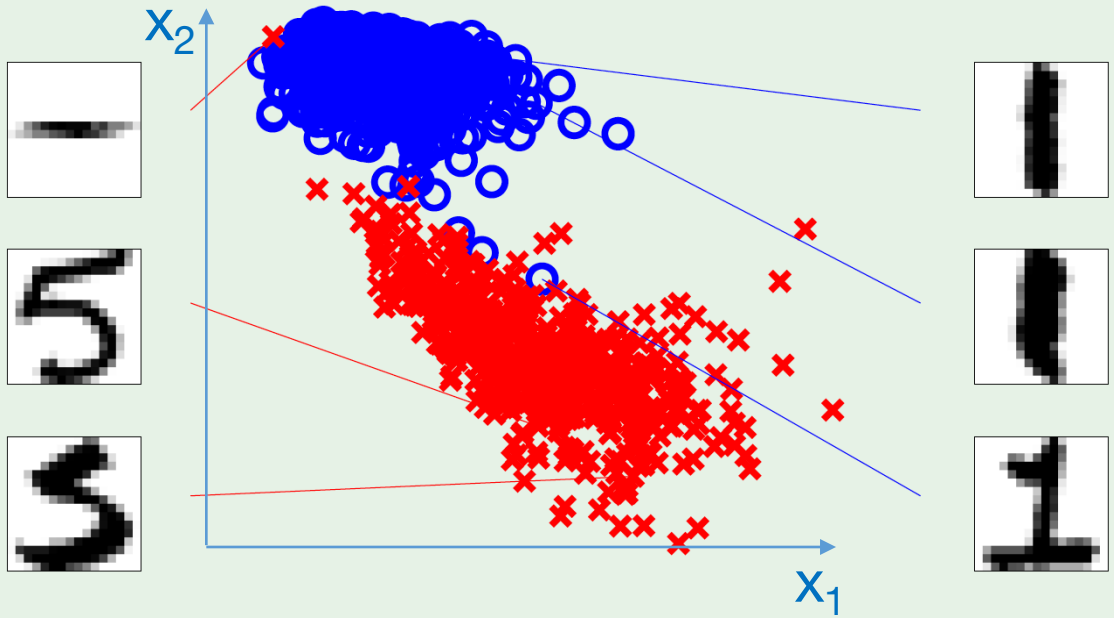


What we need for network testing:

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

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

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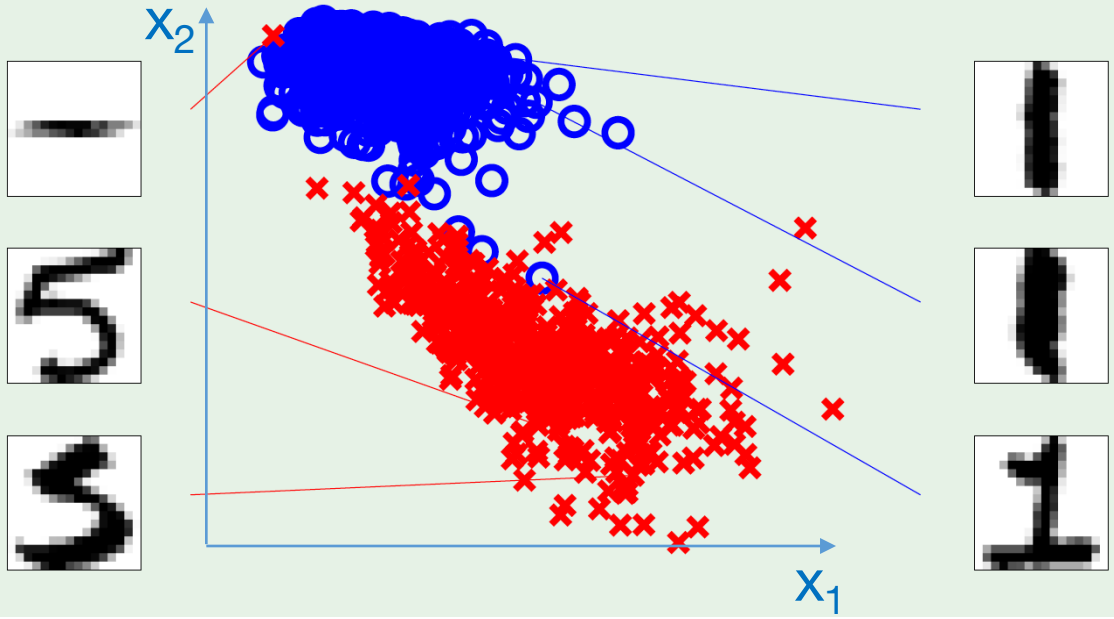


Linear classification:

Use MSE error model

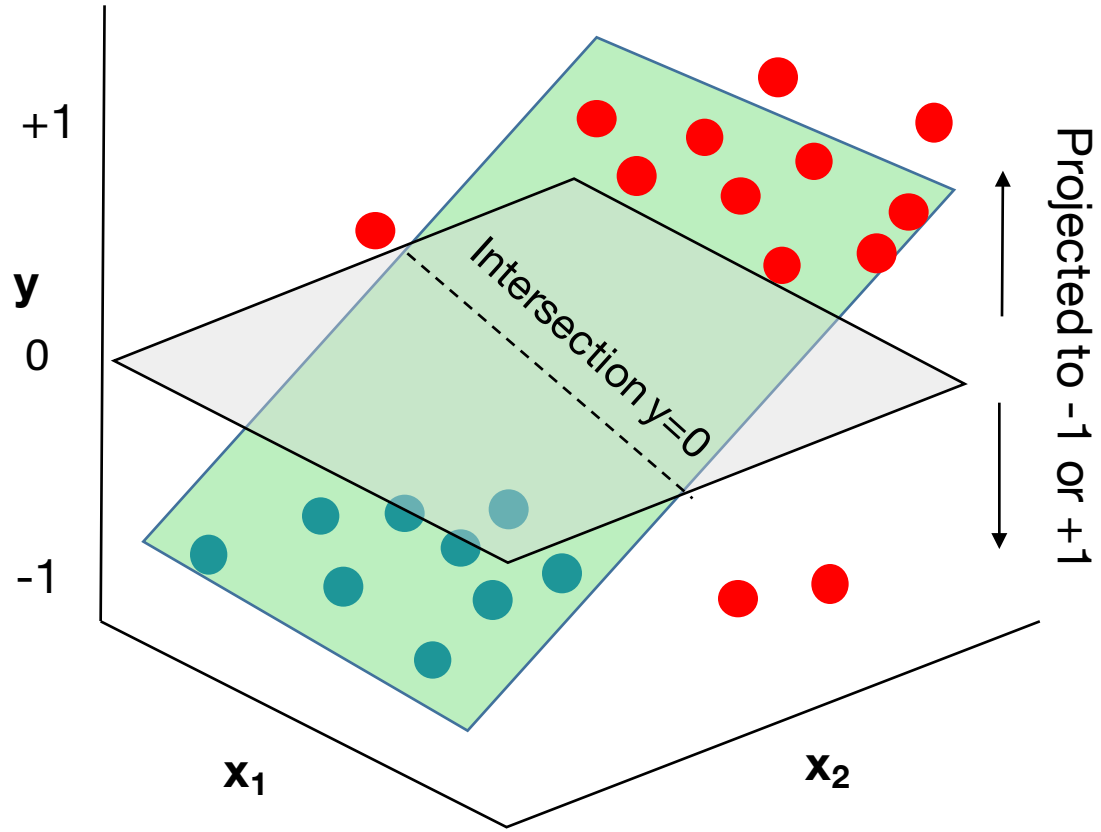
$$L = \frac{1}{N}\sum_{i=1}^{N}(w^T x_i - y_i)^2$$

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?



With sgn() operation:

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- 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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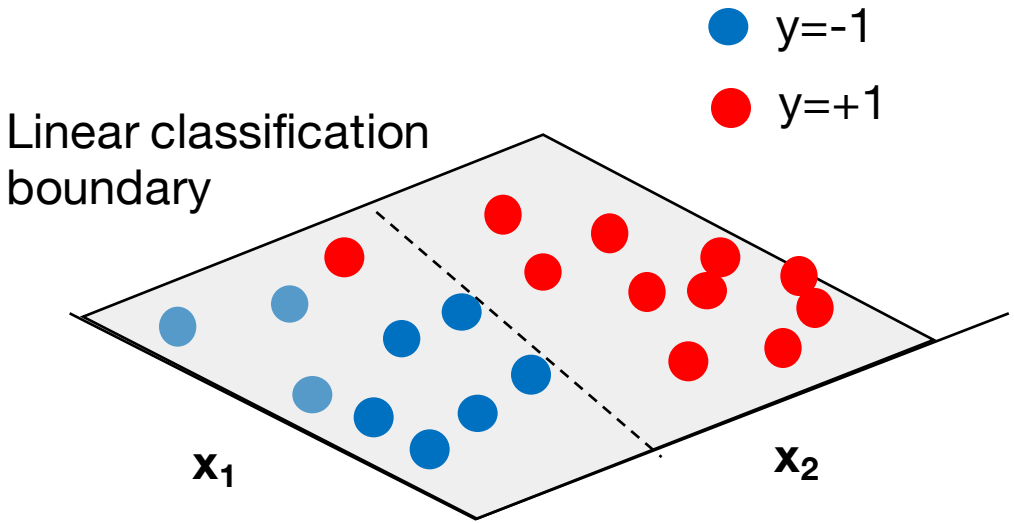

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Closed-form solution available for this line of best fit **w** via pseudo-inverse (see last lecture's notes)

Let's consider some other strategies to solve for **w**...

Simplest gradient descent: numerically compute the gradient and take a step

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

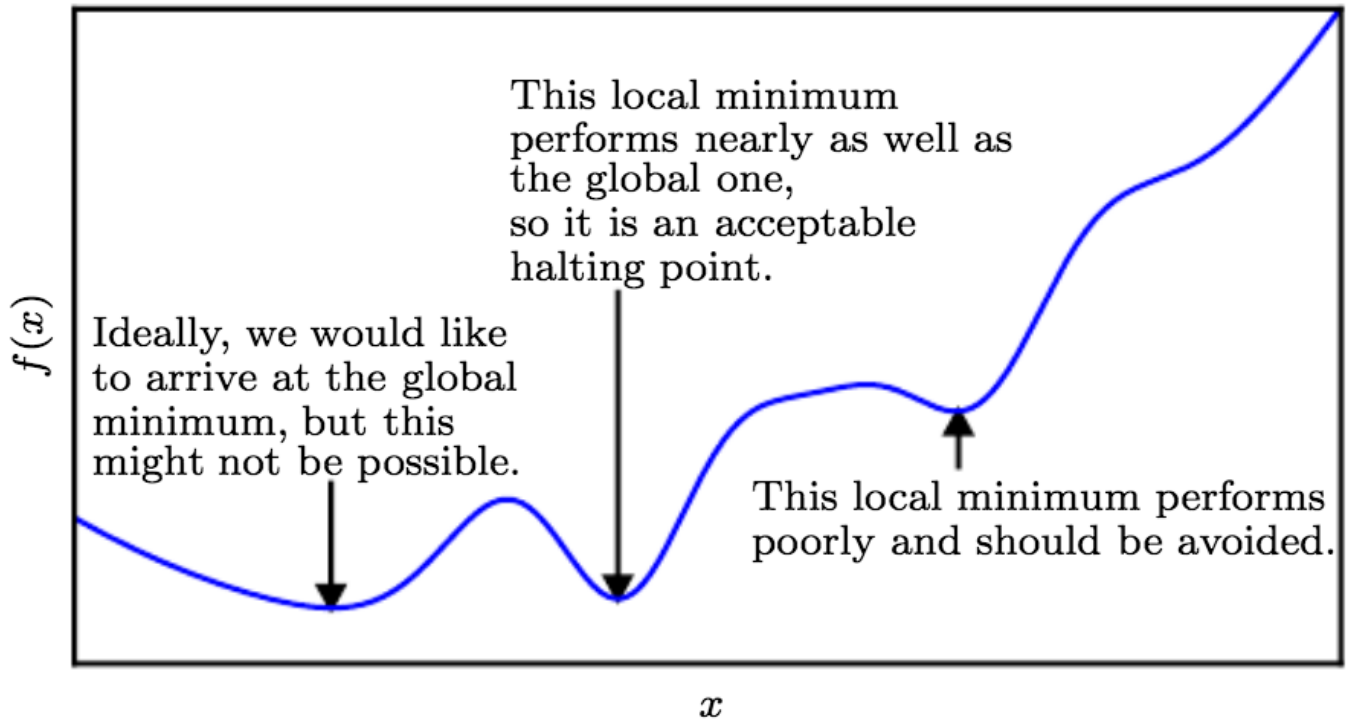
$dL(W_1)/dW_1$ = 10

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

Some quick details about gradient descent

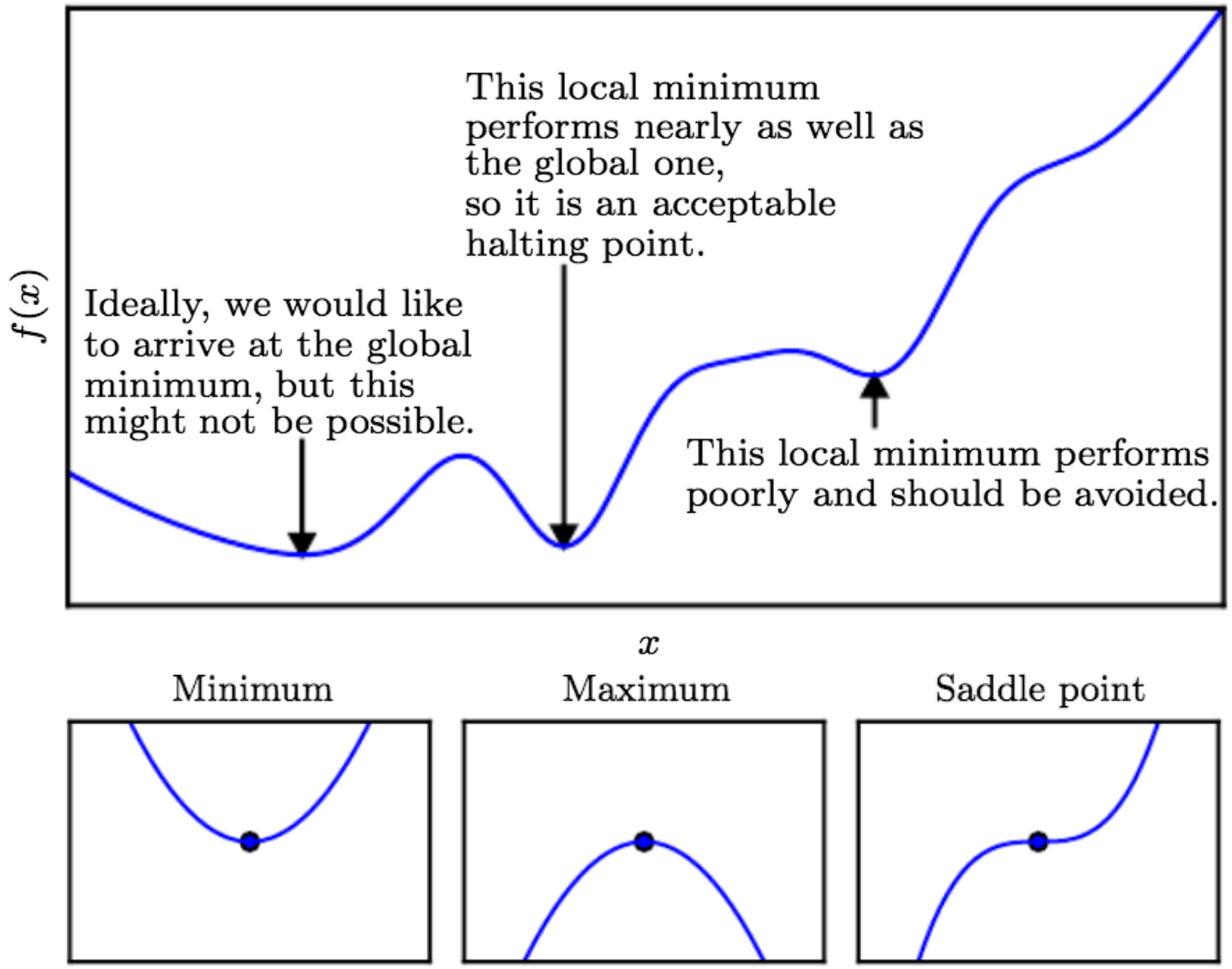
deep imaging

- For non-convex functions, local minima can obscure the search for global minima
- Analyzing critical points (plateaus) of function of interest is important



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

$f : \mathbb{R}^n \rightarrow \mathbb{R}$ (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:** $\nabla_{\boldsymbol{x}} f(\boldsymbol{x})$

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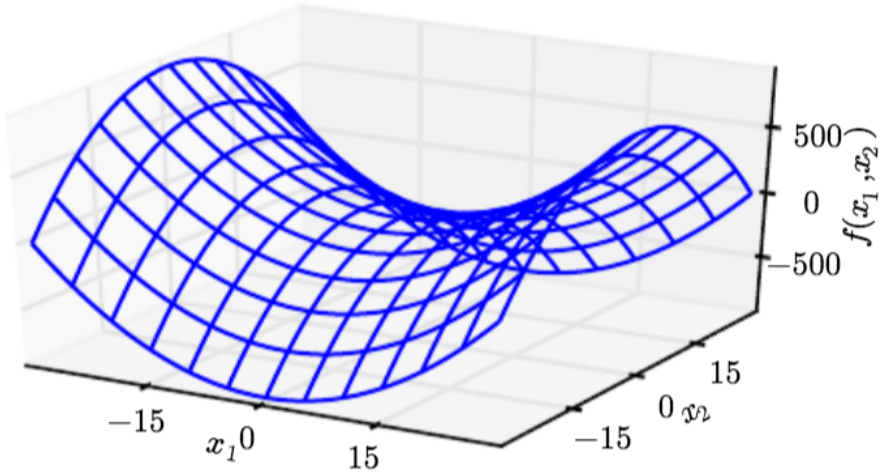
In general, we'll have functions that map m variables to n variables

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

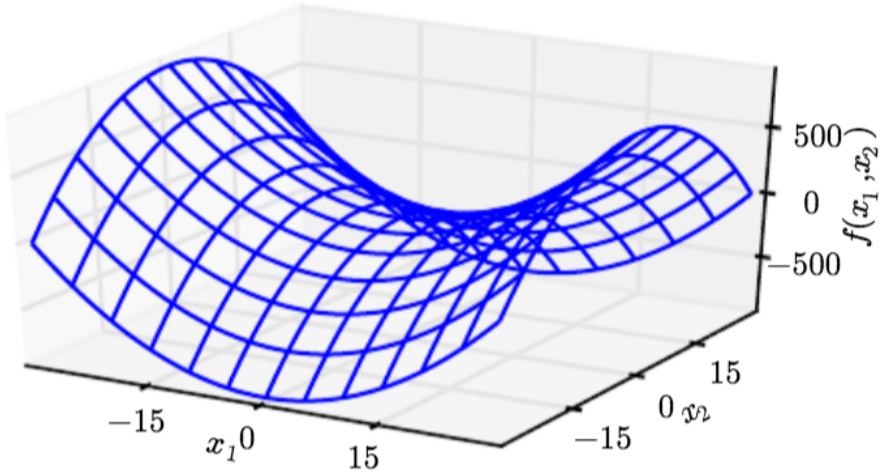
$\boldsymbol{J} \in \mathbb{R}^{n \times m}$ of $\boldsymbol{f}$: $J_{i,j} = \frac{\partial}{\partial x_j} f(\boldsymbol{x})_i$ Jacobian Matrix

Quick example



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

Quick example



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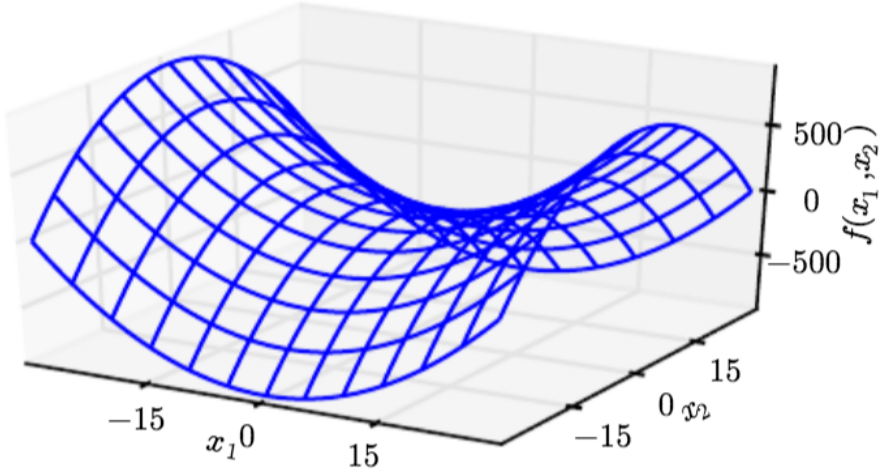
$$g = \begin{bmatrix} 2x_1 \\ -2x_2 \end{bmatrix}$$

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

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

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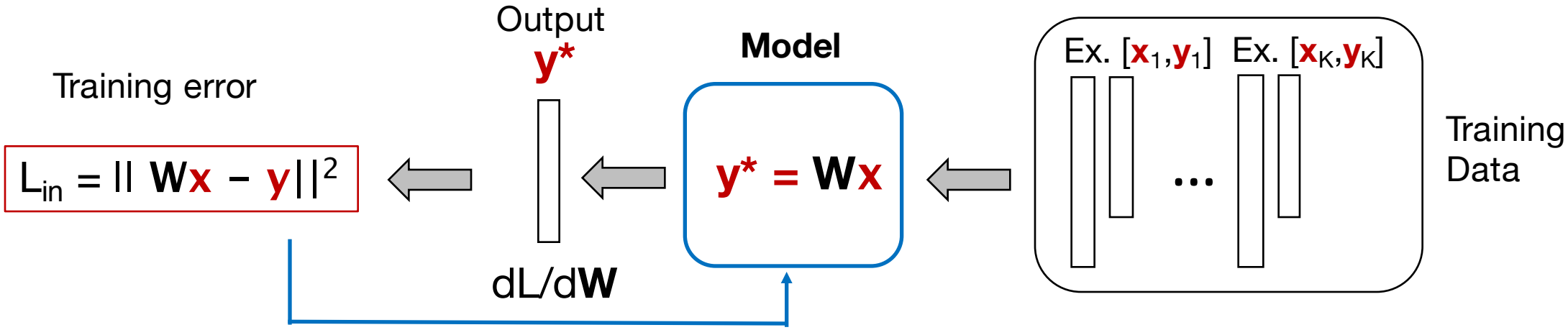
Solve for optimal step (when Hessian is positive): $\boxed{\epsilon^* = \frac{\boldsymbol{g}^\top \boldsymbol{g}}{\boldsymbol{g}^\top \boldsymbol{H} \boldsymbol{g}}}$

The linear classification model – what's not to like?



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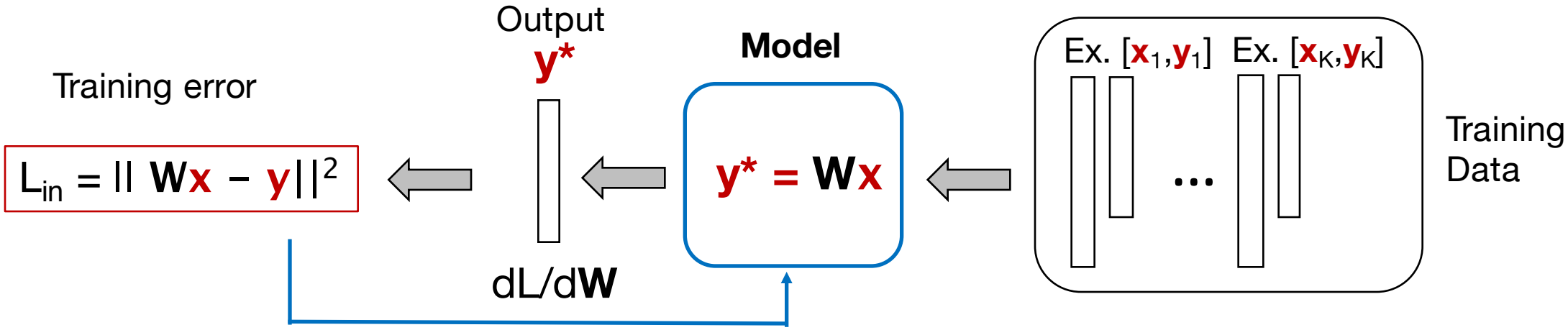

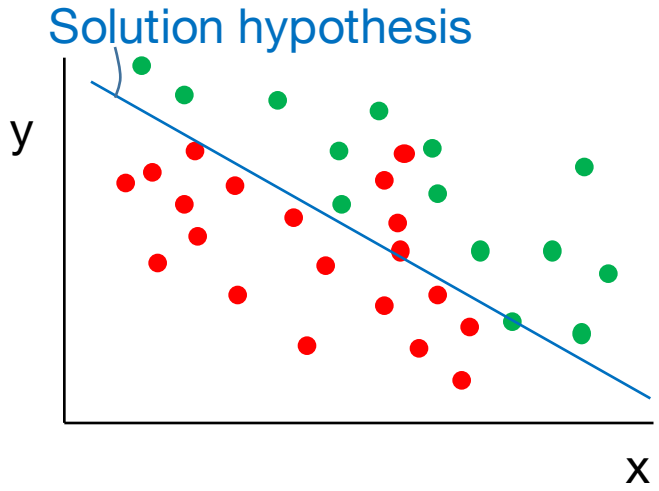

1. Can only separate data with lines (hyper-planes)…

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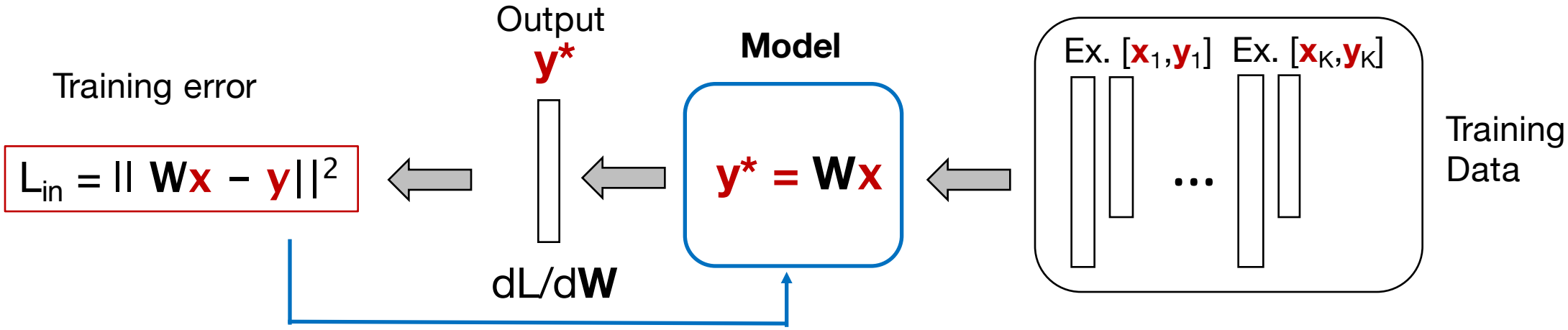

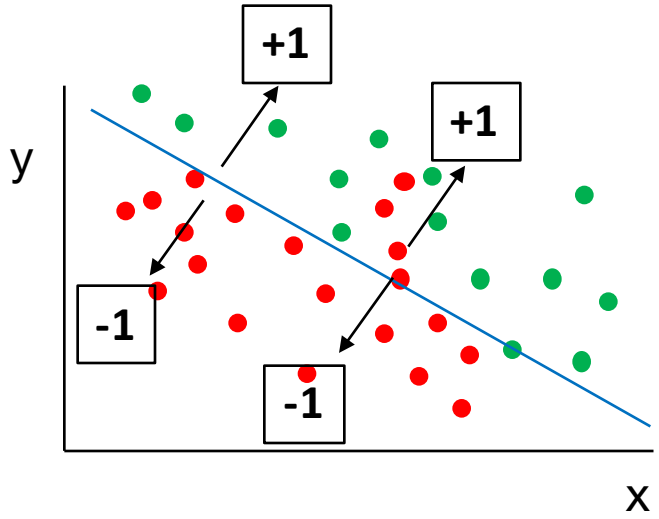

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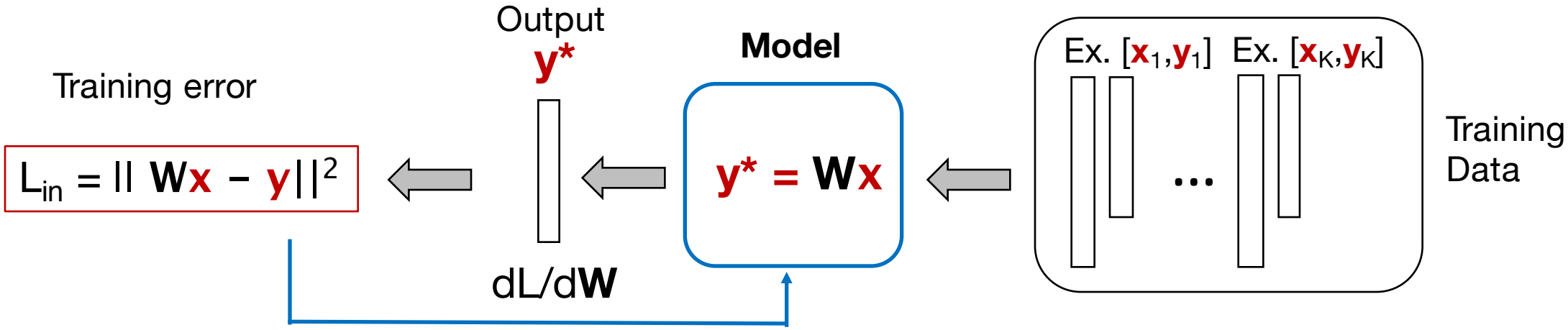
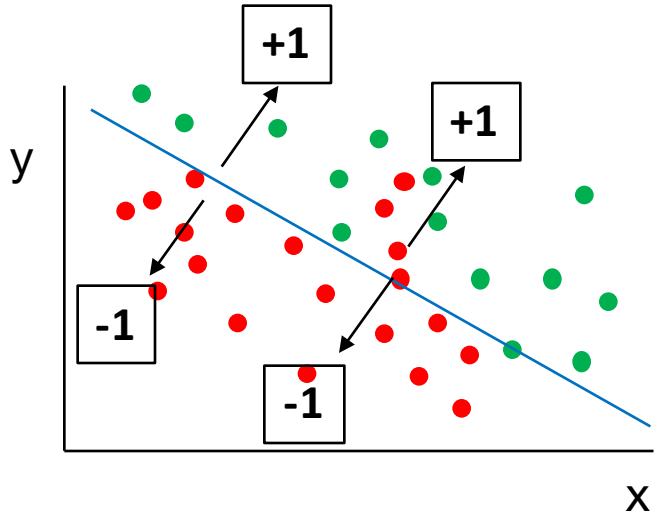
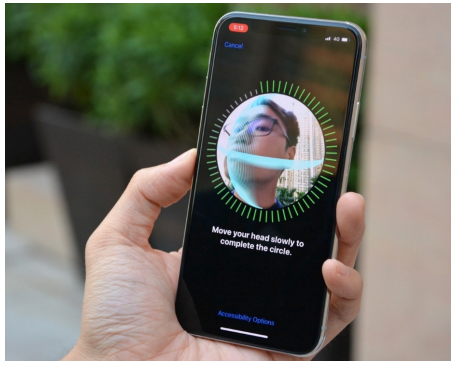
The linear classification model – what's not to like?



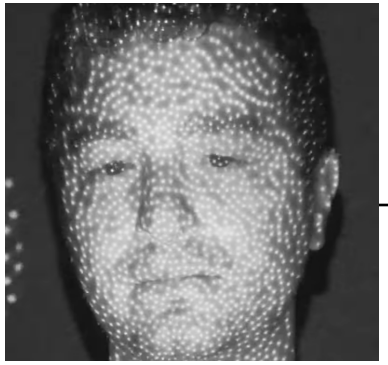


1. Can only separate data with lines (hyper-planes)…
2. We only allowed for binary labels (y = +/- 1)
3. Error function L_{in} inherently makes assumptions about statistical distribution of data

Cost functions matter: a simple example



x



f(x, W)

+1 = You

-1 = Bad guy

https://www.cnet.com/how-to/apple-face-id-everything-you-need-to-know/

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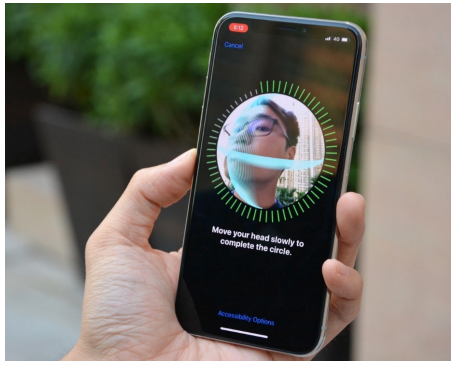

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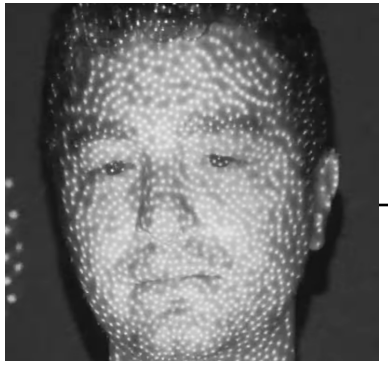

f(x, W) → +1 = You

-1 = Bad guy

Two types of error: false accept and false reject

f(x, W)

y	+1	-1
+1	No Error (you/you)	False reject
-1	False accept	No Error (bad guy/ bad guy)

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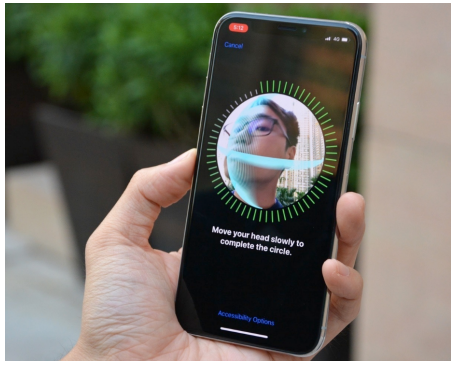
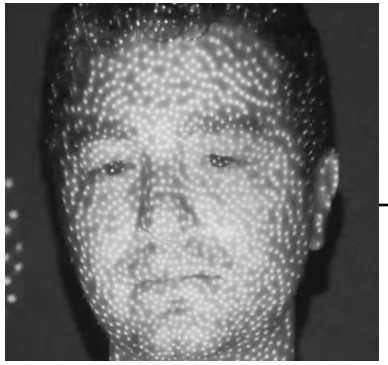
Cost functions matter: a simple example



x



f(x, W) → +1 = You, -1 = Bad guy

Two types of error: false accept and false reject

On a standard phone, what's a good cost function?

f(x, W)

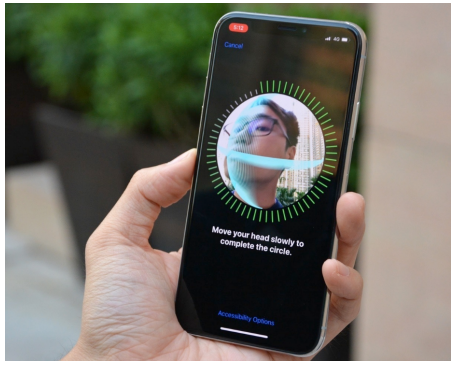
y \ f(x, W)	+1	-1
+1	No Error	False reject
-1	False accept	No Error

It's you, but you can't get in…

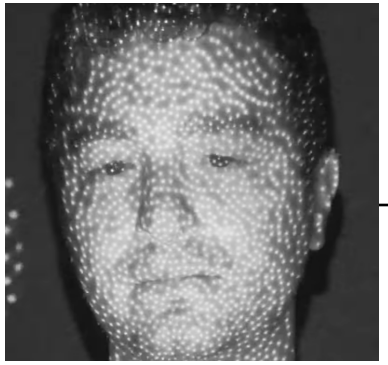
Letting an intruder in

https://www.cnet.com/how-to/apple-face-id-everything-you-need-to-know/

Cost functions matter: a simple example



x



f(x, W) → +1 = You, -1 = Bad guy

Two types of error: false accept and false reject

On a standard phone, what's a good cost function?

$$L_{in} = \text{ReLU}[f(x, W)-y] + \mathbf{10}\ \text{ReLU}[y-f(x, W)]$$

Penalty for intruder

Large penalty for annoyance…

f(x, W)

y \ f(x, W)	+1	-1
+1	No Error	False reject
-1	False accept	No Error

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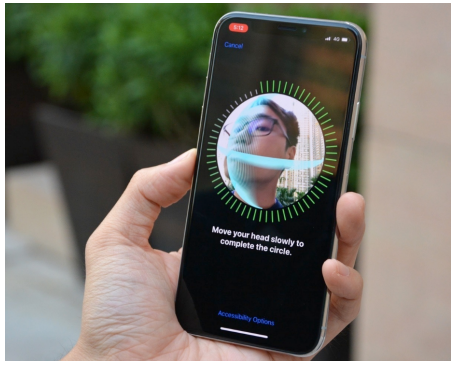

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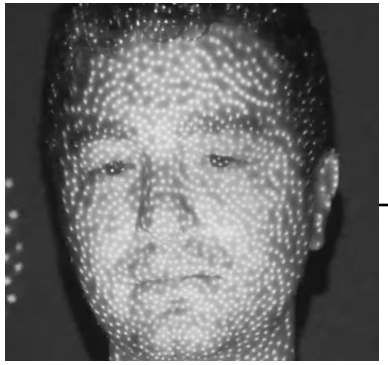

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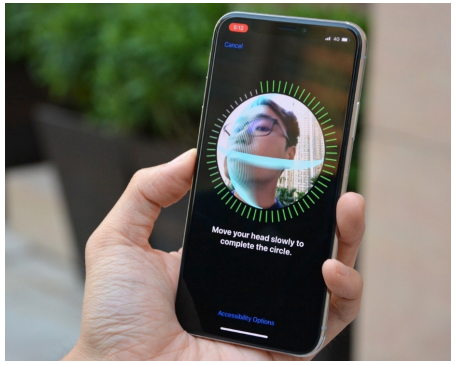

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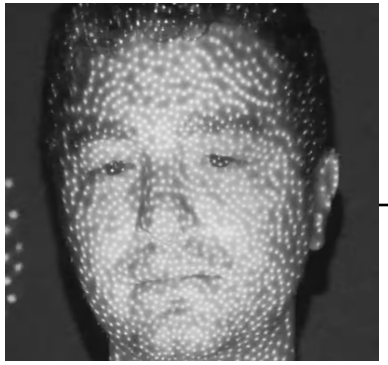

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BIG penalty for intruder

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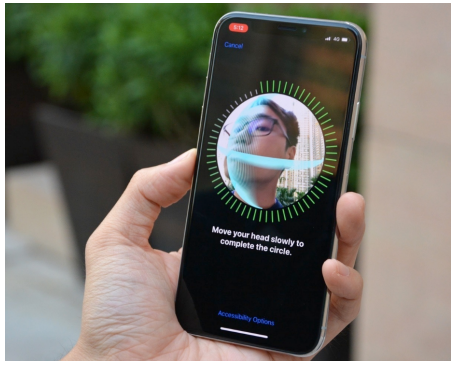

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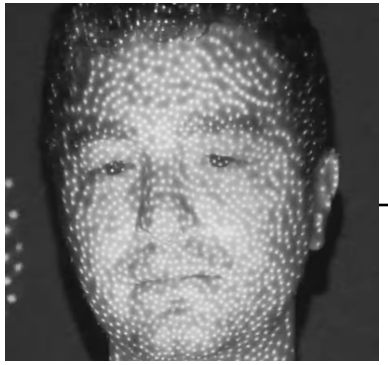

f(x, W) → +1 = You

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Establishing cost function tied to conditional probabilities:

$P(y = -1 \mid f(x,W) = +1)$

$P(y = +1 \mid f(x,W) = -1)$

Establish L, W to balance these probabilities

f(x, W)

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Machine learning and probability

- Probability measures help determine when to use certain cost functions
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$$p(\mathbf{w}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{x})}$$

With 2 conditioned variables:

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$$p(\mathbf{w}|\mathbf{x},\mathbf{y}) \propto p(\mathbf{x},\mathbf{y}|\mathbf{w}) \propto p(\mathbf{y}|\mathbf{x},\mathbf{w})$$

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What you want: but hard to vary data to find model…

$$p(\mathbf{w}|\mathbf{x},\mathbf{y}) \propto p(\mathbf{x},\mathbf{y}|\mathbf{w}) \propto p(\mathbf{y}|\mathbf{x},\mathbf{w})$$

What you can do: test the model, check the result

Linear classification is the maximum likelihood for Gaussian data

- Given a close relationship between $p(\mathbf{w}|\mathbf{x}, \mathbf{y}) \longleftrightarrow p(\mathbf{y}|\mathbf{x}, \mathbf{w})$:

  Maximum likelihood estimation asks the question,

$$\text{For what } \mathbf{w} \text{ is } p(\mathbf{y}_1, \ldots \mathbf{y}_N | \mathbf{x}_1, \ldots \mathbf{x}_N; \mathbf{w}) \text{ maximized?}$$

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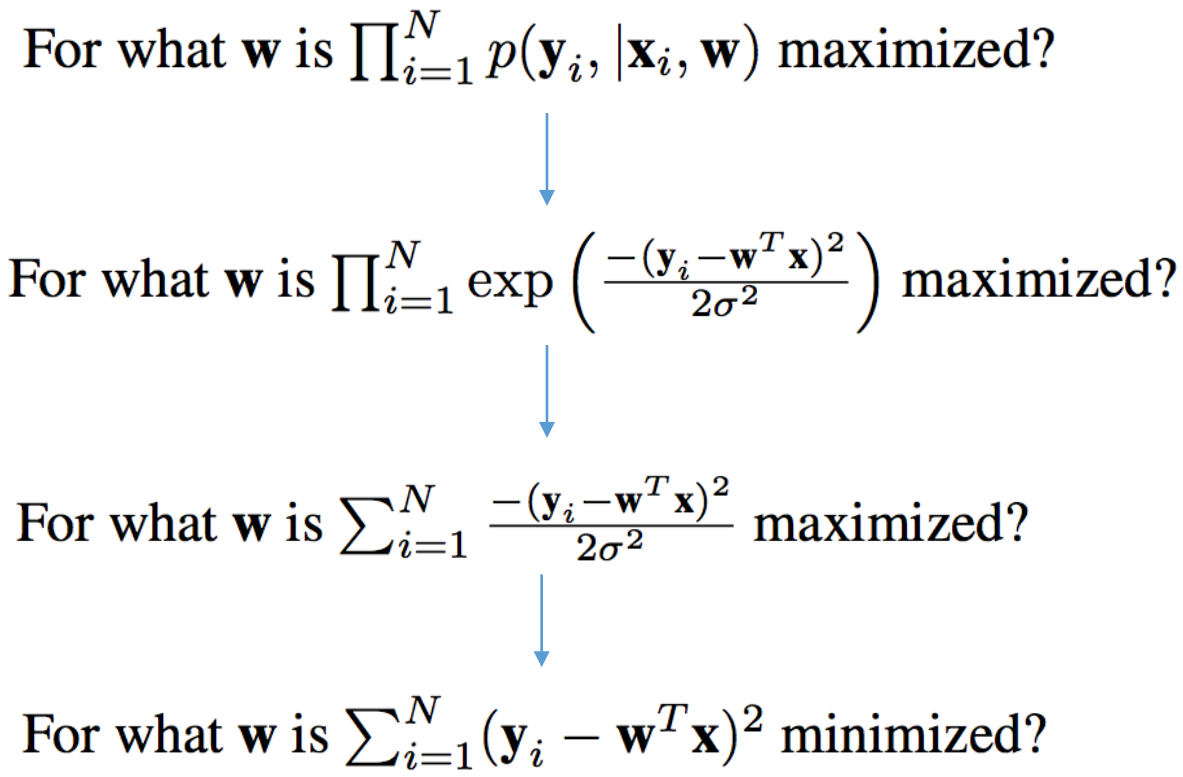
- Let's assume our labels are a "noisy" Gaussian process that surround the correct label:

$$y_i = \mathbf{w}^T \mathbf{x}_i + n \qquad (n \text{ is zero-mean Gaussian noise})$$

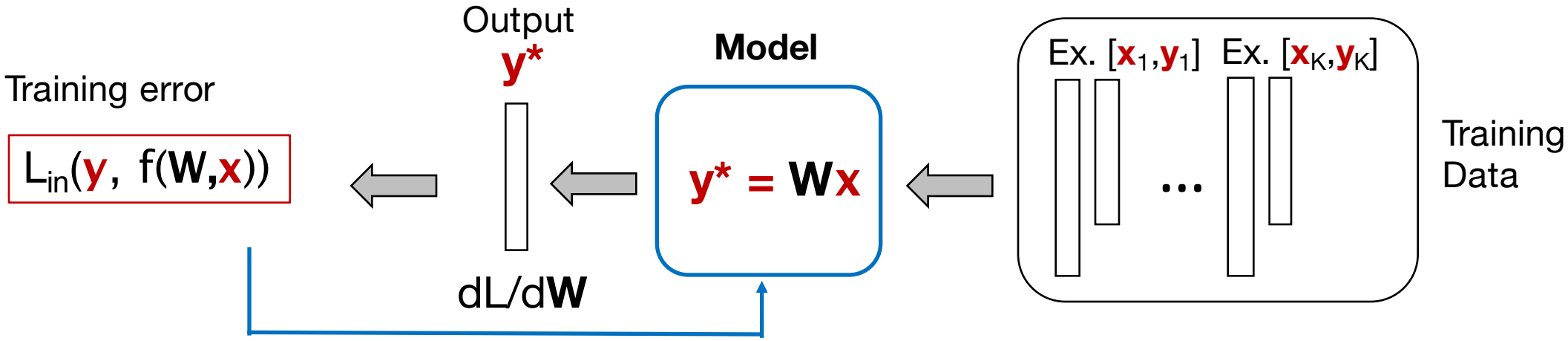
- Then, the above cond. prob. for labels can be expressed as a multivariate Gaussian

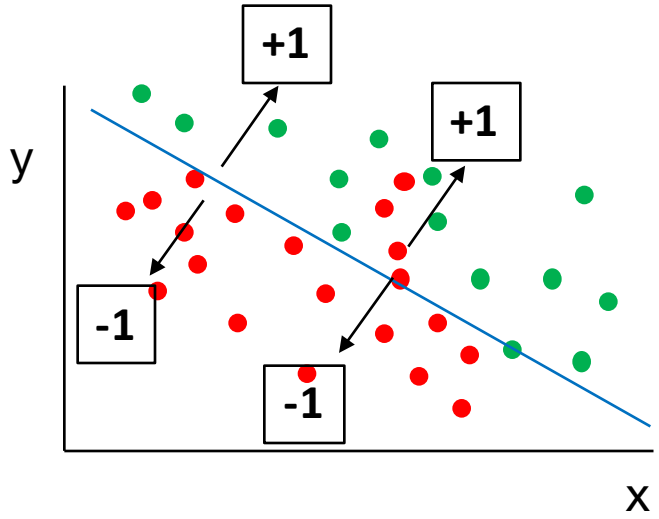
Linear classification is the maximum likelihood for Gaussian data



Summary: Linear classification assumes labels are a Gaussian random process, and then thresholds them to ether -1 or +1

The linear classification model – what's not to like?





1. Can only separate data with lines (hyper-planes)…
2. We only allowed for binary labels (y = +/- 1)
3. Error function L_{in} inherently makes assumptions about statistical distribution of data

Let's think about the labels as a probabilistic measure:

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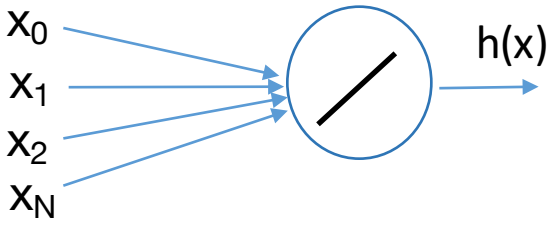
Linear regression:

$$h(x) = x \in (-\infty, \infty)$$

Linear regression



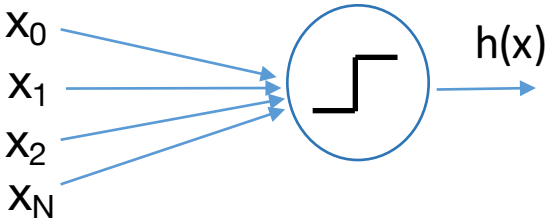
Not a probabilistic mapping

Linear classifier:

$$h(x) = \text{sign}(w_o^T x_j)$$

$$h(x) = \text{sign}(x) \in \{0, 1\}$$

Sign(x)



Probabilistic, but all-or-nothing

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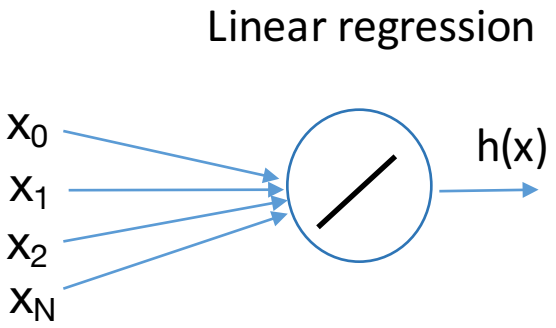

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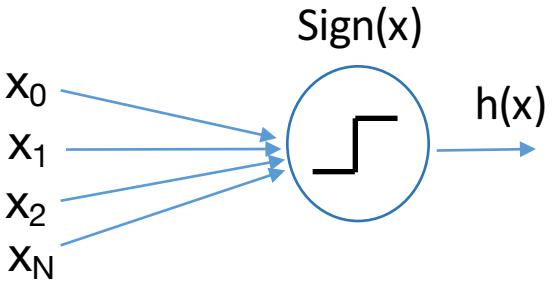

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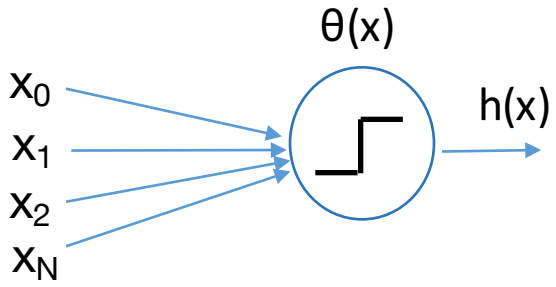
Logistic classifier:

$$h(x) = \theta(\,x) \in \; [0,\, 1]$$



Probabilistic

Probabilistic interpretation of function that maps outputs to labels, $h(x) = \theta(x)$

Example: You are trying to predict the probability that a patient may have a certain form a disease, $\theta(\mathbf{x})$, given a number of observations and measurements, $\mathbf{x}$

Example: You are trying to predict the probability of rain tomorrow, $\theta(\mathbf{x})$, given a set of satellite image data, $\mathbf{x}$

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Example: You are trying to predict the probability that a patient may have a certain form a disease, θ(**x**), given a number of observations and measurements, **x**

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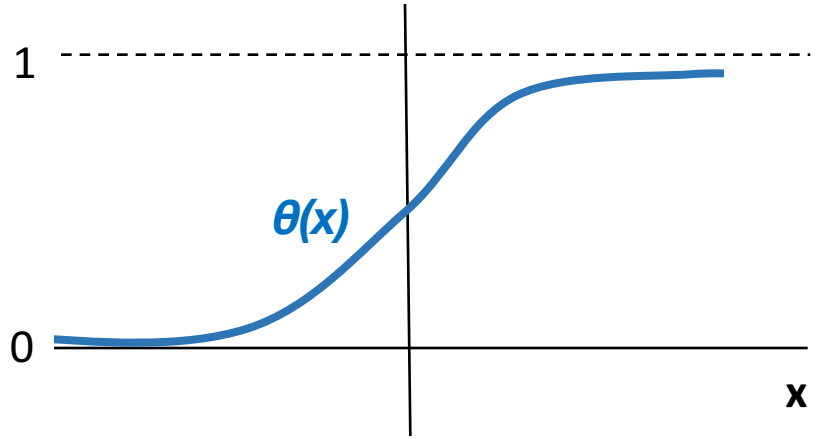
The Logistic Function *θ*

$$\theta(x) = \frac{e^x}{1+e^x}$$

Also called Sigmoid function



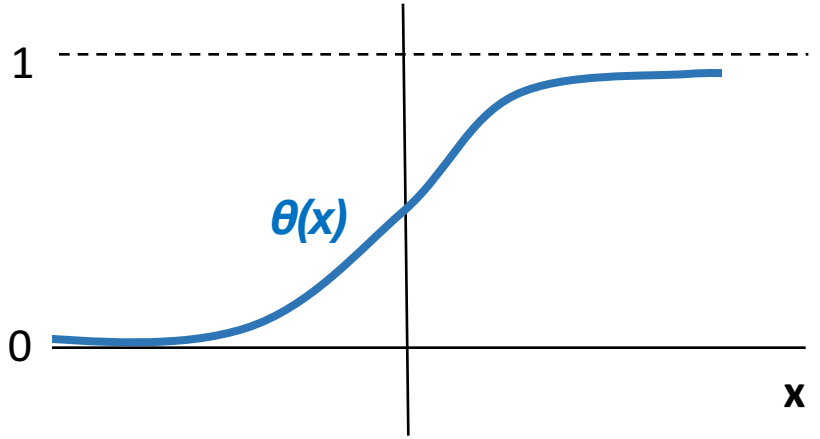
- Use soft threshold to map any number to [0,1] range
- Sigmoid "flattens out" x

From linear classification to logistic classification

- Let's re-derive a cost function for the case where labels are treated as probabilities
  - You'll use derivatives of this more often than not in Tensorflow
- During learning, we will again have two classes (in this simple example), y= +/- 1
- map these binary values onto a [0,1] probability distribution

Formula for likelihood using the logistic function θ, given binary labels

$$P(y \mid \mathbf{x}) = \begin{cases} \theta(f(\mathbf{x})) & \text{For } y = +1 \\ 1 - \theta(f(\mathbf{x})) & \text{For } y = -1 \end{cases}$$



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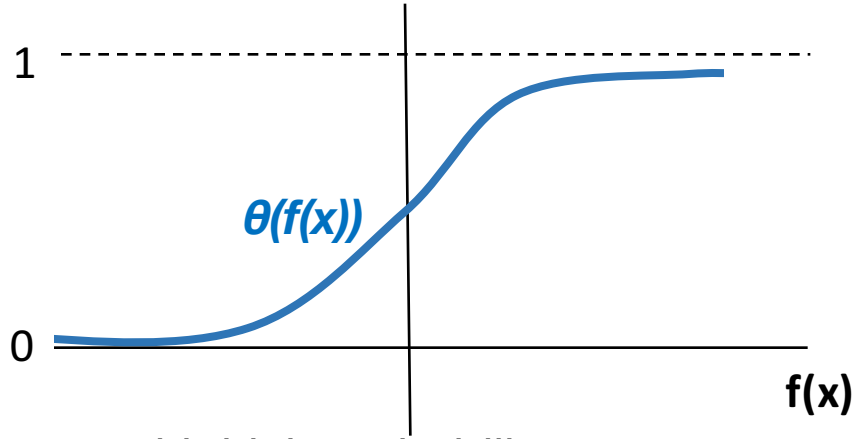


Rough Interpretation:

- If network output f(x) is large, then should map to y=+1 with high probability
- θ(f(x)) is large for large value of x
- If network output f(x) is small, then should map to y=-1 with high probability
- θ(f(x)) ~0 for small values of f(x), so 1- θ(f(x)) ~1 is high probability to y=-1 mapping

Deriving cost function for logistic classification for probabilistic outputs

Instead of mapping f(**x**) to either +1 or -1 with the sign operator, let's use θ to map it to lie between 0 and 1:

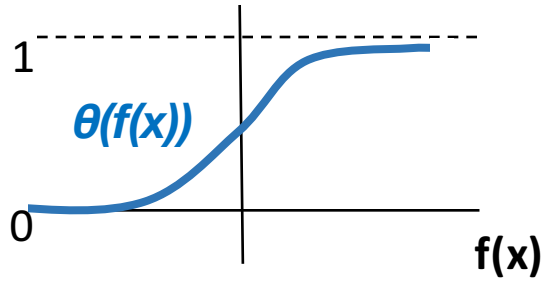
$$P(y \mid \mathbf{x}) = \begin{cases} \theta(f(\mathbf{x})) & \text{For } y = +1 \\ 1 - \theta(f(\mathbf{x})) & \text{For } y = -1 \end{cases}$$

We'll stick with the case of linear classification, where $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$

Also, please note that for the logistic function, θ(-a) = 1 - θ(a). So, we can summarize the case-based definition above with a single function,

$$P(y \mid \mathbf{x}) = \theta(y\, \mathbf{w}^T\mathbf{x})$$

Where y = +/-1 flips $\theta(\mathbf{w}^T\mathbf{x})$ to be either $\theta(\mathbf{w}^T\mathbf{x})$ or $\theta(-\mathbf{w}^T\mathbf{x}) = 1 - \theta(\mathbf{w}^T\mathbf{x})$



Deriving cost function for logistic classification for probabilistic outputs

Similar to the linear classification case, the likelihood of observing *N* independent outputs is given by,

$$P(y_1, y_2 \ldots y_N \mid \mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n) = \prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n)$$

$$= \prod_{n=1}^{N} \theta(y_n \, \mathbf{w}^T \mathbf{x}_n)$$

This is the probability of the labels, given the data. We'd like to maximize this probability!

*Like the linear regression case, but now the probability of classes given the data is not Gaussian distributed, but instead follows the sigmoid curve (is bound to [0,1], which is more realistic)

$$\text{Maximize} \quad P(y_1, y_2 \ldots y_N \mid \mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n \, \mathbf{w}^T \mathbf{x}_n)$$

Deriving cost function for logistic classification for probabilistic outputs

Maximize $P(y_1, y_2 \ldots y_N \mid \mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n \mathbf{w}^T \mathbf{x}_n)$

Minimize $$-\frac{1}{N} \ln \left(\prod_{n=1}^{N} \theta(y_n \mathbf{w}^T \mathbf{x}) \right)$$

Minimize $$\frac{1}{N} \sum_{n=1}^{N} \ln \left(\frac{1}{\theta(y_n \mathbf{w}^T \mathbf{x})} \right)$$

Use relationship $$\theta(a) = \frac{1}{1 + e^{-a}}$$

Minimize $$L_{in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \ln(1 + e^{-y_n \mathbf{w}^T \mathbf{x}})$$

Cross entropy error for logistic classification

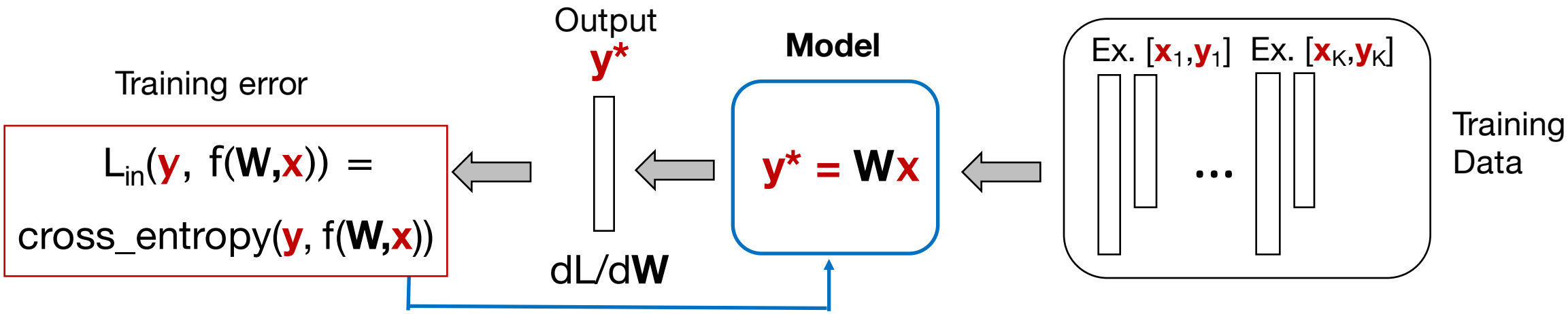
Requires iterative solution to minimize

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

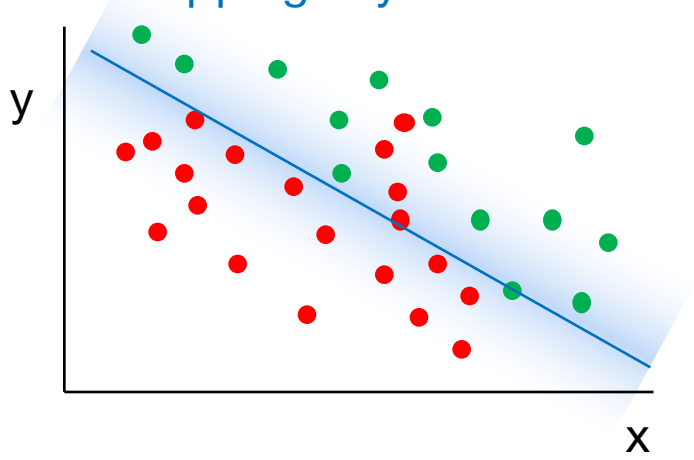
Mean-square error for linear classification

Closed form solution available

The linear classification model – what's not to like?



Probabilistic mapping to y



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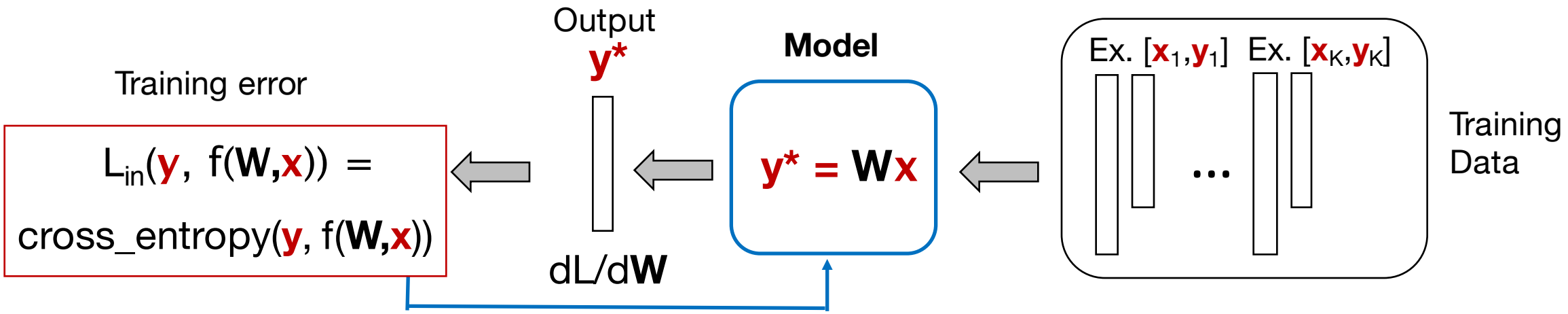

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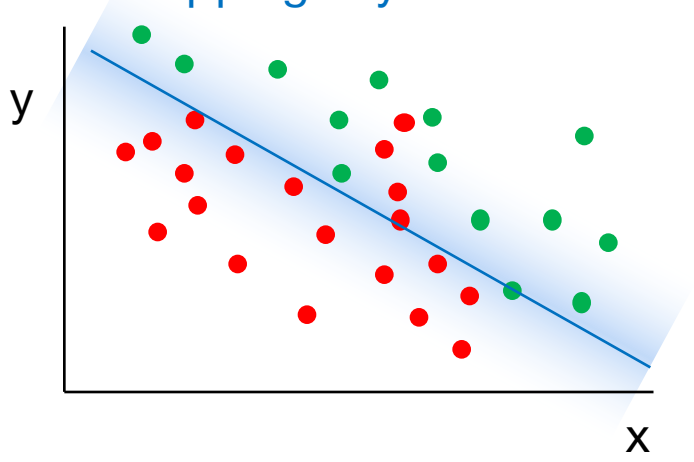

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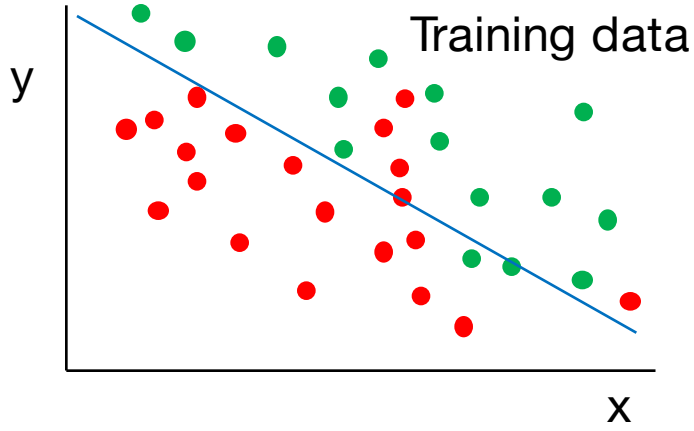
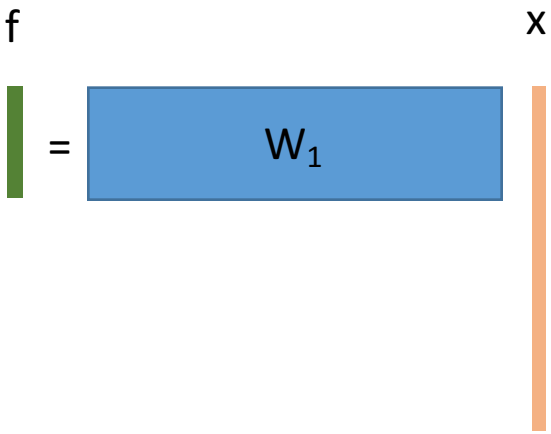
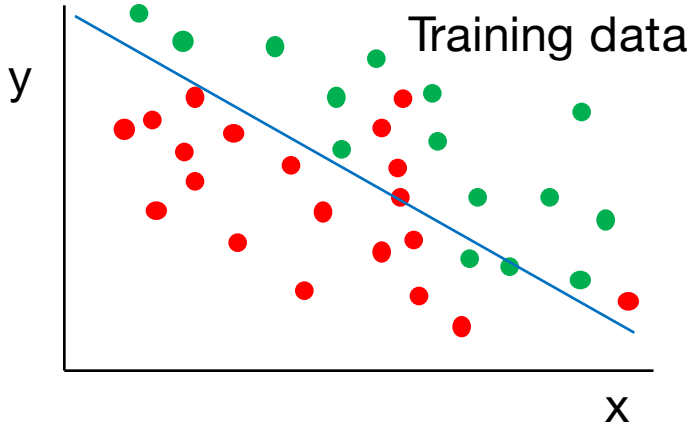


$$f = W_1 x$$

Learned *f:* not flexible

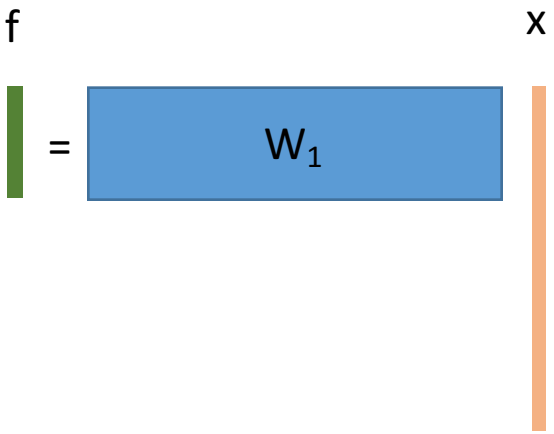


deep imaging



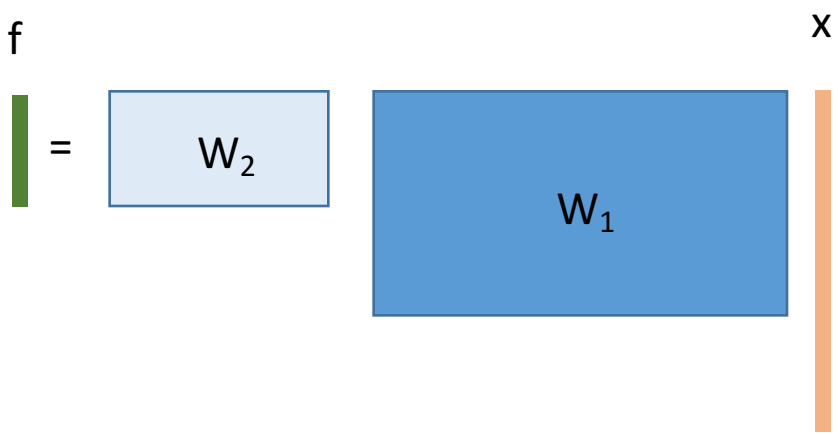
$$f = W_1 x$$

Learned *f:* not flexible



Can we add flexibility by multiplying with another weight matrix?

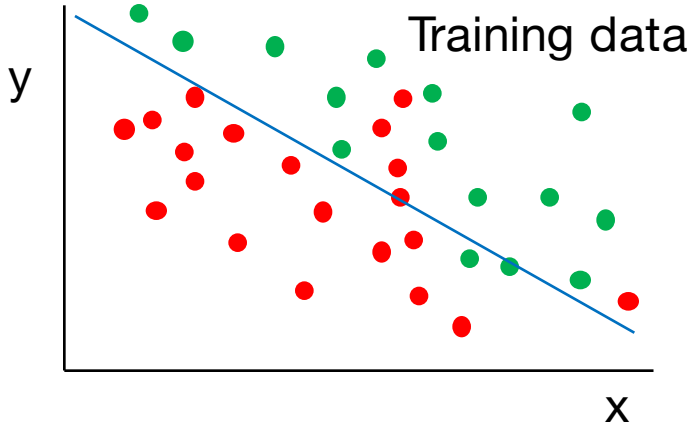
$$\begin{cases} f_1 = W_1 x + b_1 \\ f_2 = W_2 f_1 + b_2 \end{cases}$$



$$f_2 = W_2(W_1 x + b_1) + b_2$$

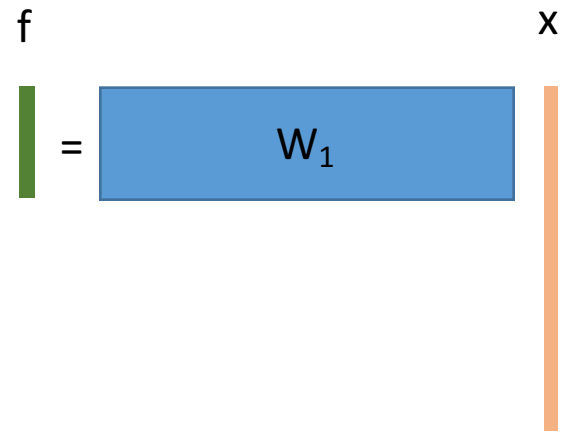
$$f_2 = W' x + b'$$

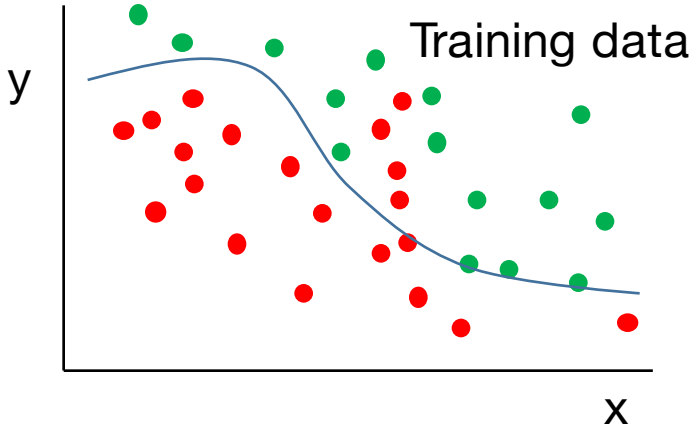
Unfortunately not…



$$f = W_1 x$$

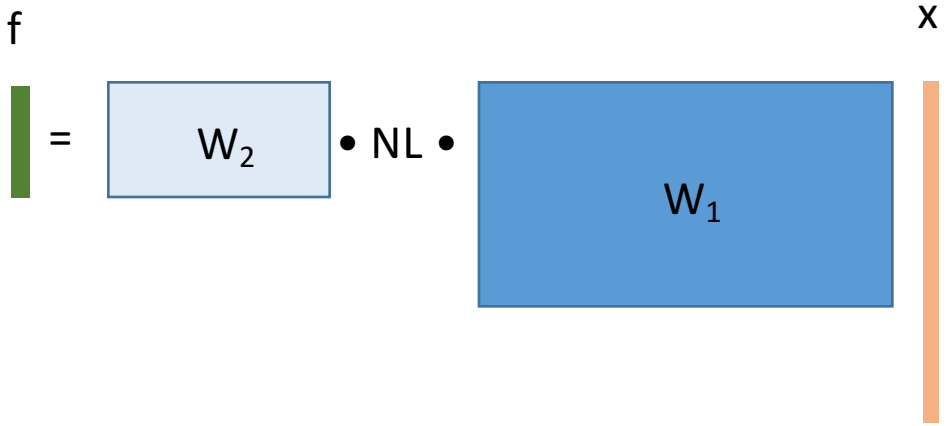
Learned *f:* not flexible

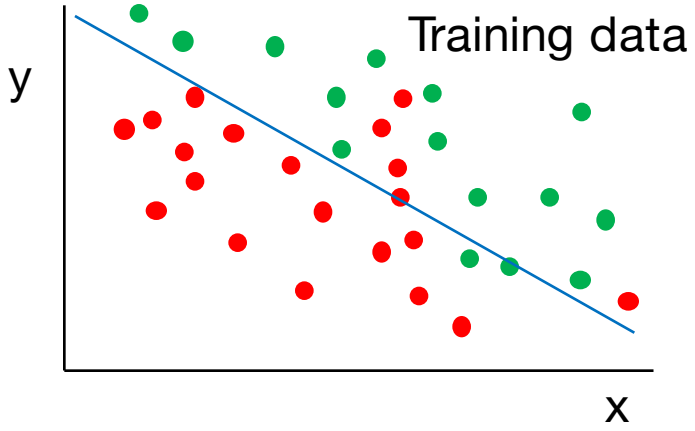




$$f = W_2 \max(W_1 x, 0)$$

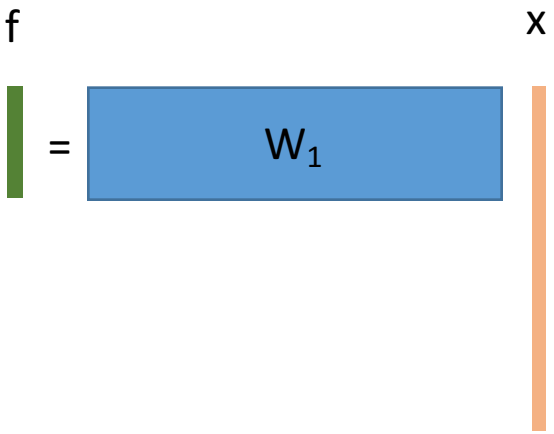
Learned *f:* a bit flexible

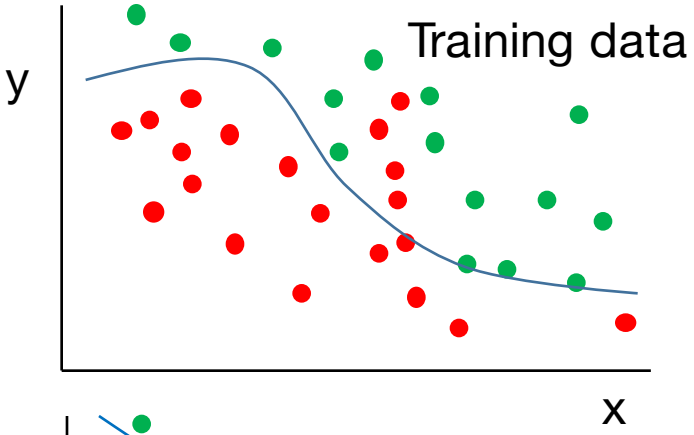




$$f = W_1 x$$

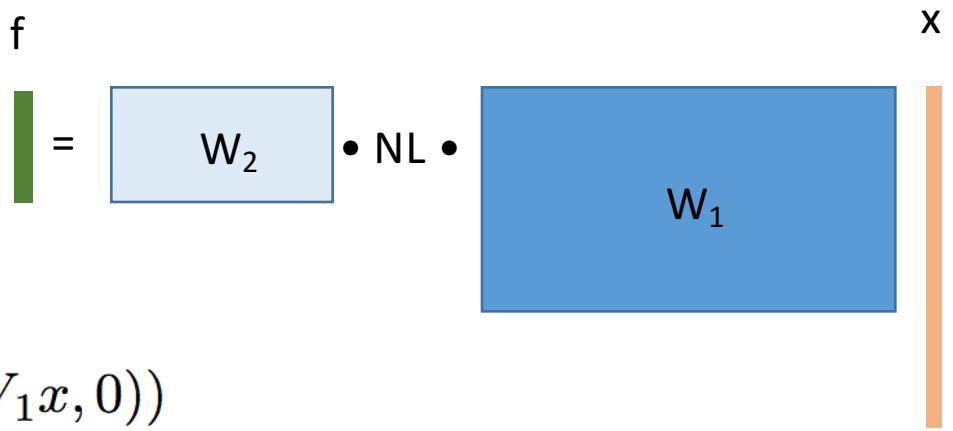
Learned *f:* not flexible

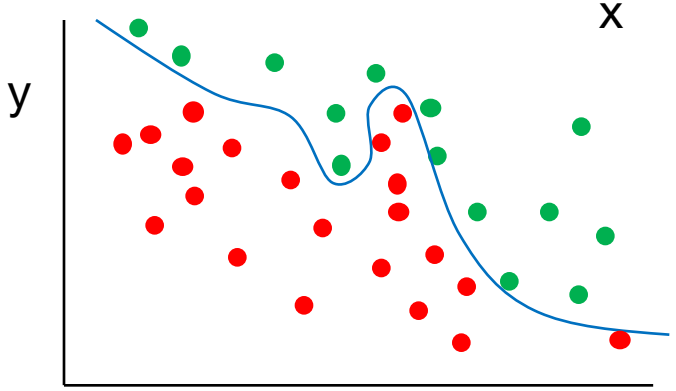




$$f = W_2 \max(W_1 x, 0)$$

Learned *f:* a bit flexible





$$f = W_3 \max(0, W_2 \max(W_1 x, 0))$$

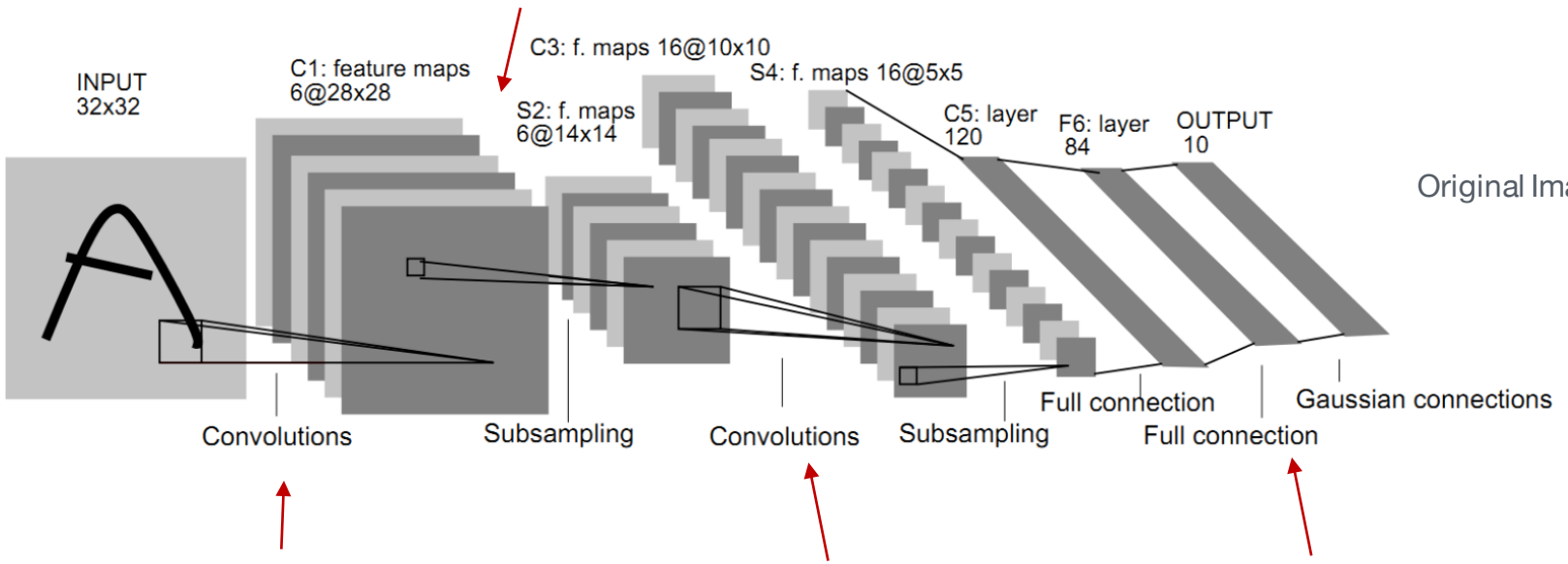
Learned *f:* more flexible

Does it generalize???

We can keep adding these “layers”…

Getting us to Convolutional Neural Networks

After, apply non-linearity and sub-sampling



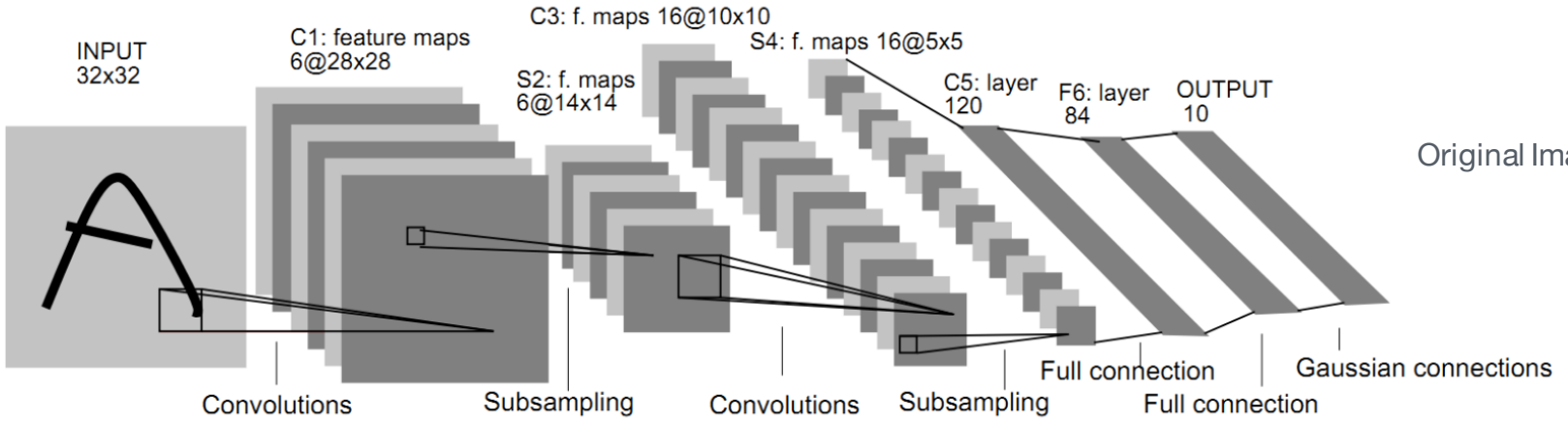
Original Image published in [LeCun et al., 1998]

Each matrix W is a convolution matrix

Repeat a few times

At the end, use a full W for a final matrix multiplication

Getting us to Convolutional Neural Networks



Original Image published in [LeCun et al., 1998]

In practice, this process is repeated many times: