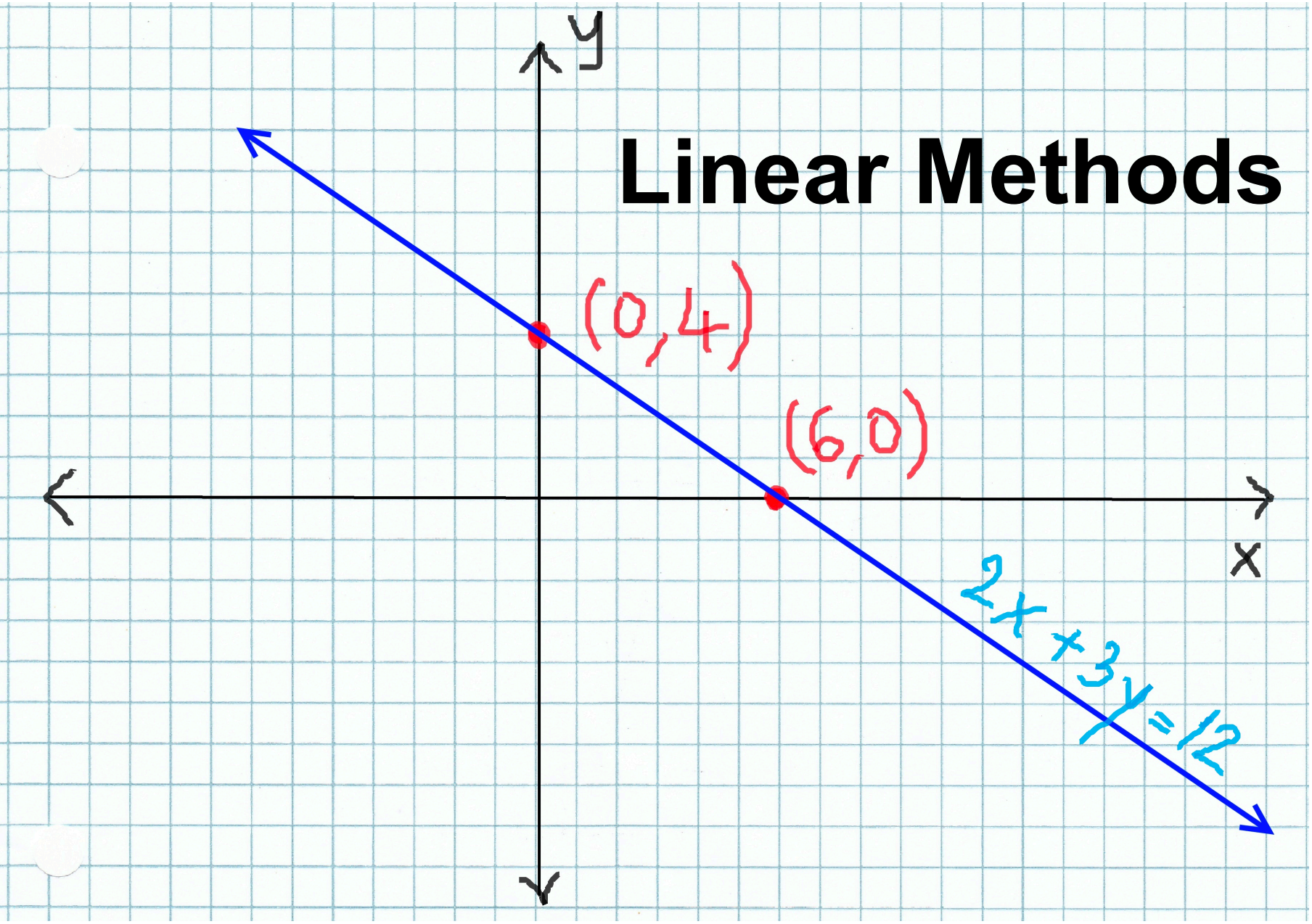
Introduction to (Deep) Learning

4. Linear Regression, Basic Optimization

slides adapted from courses.d2l.ai/berkeley-stat-157


Linear Methods
y
x
(0,4)
(6,0)
2x + 3y = 12

House Buying 101

- Pick a house, take a tour, and read facts
- Estimate its price, bid



Listing price from agent

$5,498,000 Price | **7** Beds | **5** Baths | **4,865** Sq. Ft. $1130 / Sq. Ft.

Redfin Estimate: $5,390,037 On Redfin: 15 days

Predicted sale price

slides adapted from courses [illegible] at-15

Virtual Tour
- Branded Virtual Tour
- Virtual Tour (External Link)

Parking Information
- Garage (Minimum): 2
- Garage (Maximum): 2
- Parking Description: Attached Garage, On Street
- Garage Spaces: 2

Multi-Unit Information
- # of Stories: 2

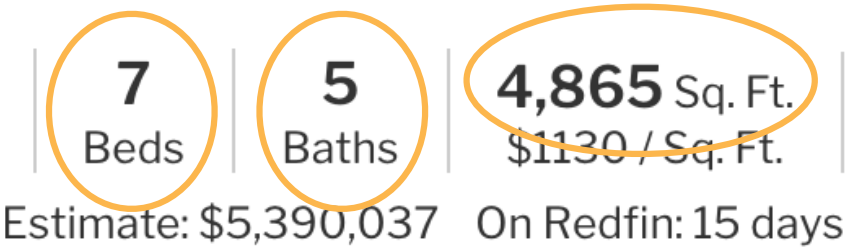
School Information
- Elementary School: El Carmelo El
- Elementary School District: Palo A
- Middle School: Jane Lathrop Stan
- High School: Palo Alto High
- High School District: Palo Alto Un

Interior Features

Bedroom Information
- # of Bedrooms (Minimum): 7
- # of Bedrooms (Maximum): 7

- Kitchen Description: Countertop (Dishwasher, Garbage Disposal, Ho Island with Sink, Microwave, Over

A Simplified Model



- Assumption 1
  The key factors impacting the prices are
  #Beds, #Baths, Living Sqft, denoted by x_1, x_2, x_3
- Assumption 2
  The sale price is a weighted sum over the key factors

$$y = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$$

  Weights and bias are determined later

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Linear Model

- Given *n*-dimensional inputs $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$
- Linear model has a *n*-dimensional weight and a bias

$$\mathbf{w} = [w_1, w_2, \ldots, w_n]^T, \quad b$$

- The output is a weighted sum of the inputs

$$y = w_1 x_1 + w_2 x_2 + \ldots + w_n x_n + b$$

Vectorized version

$$y = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

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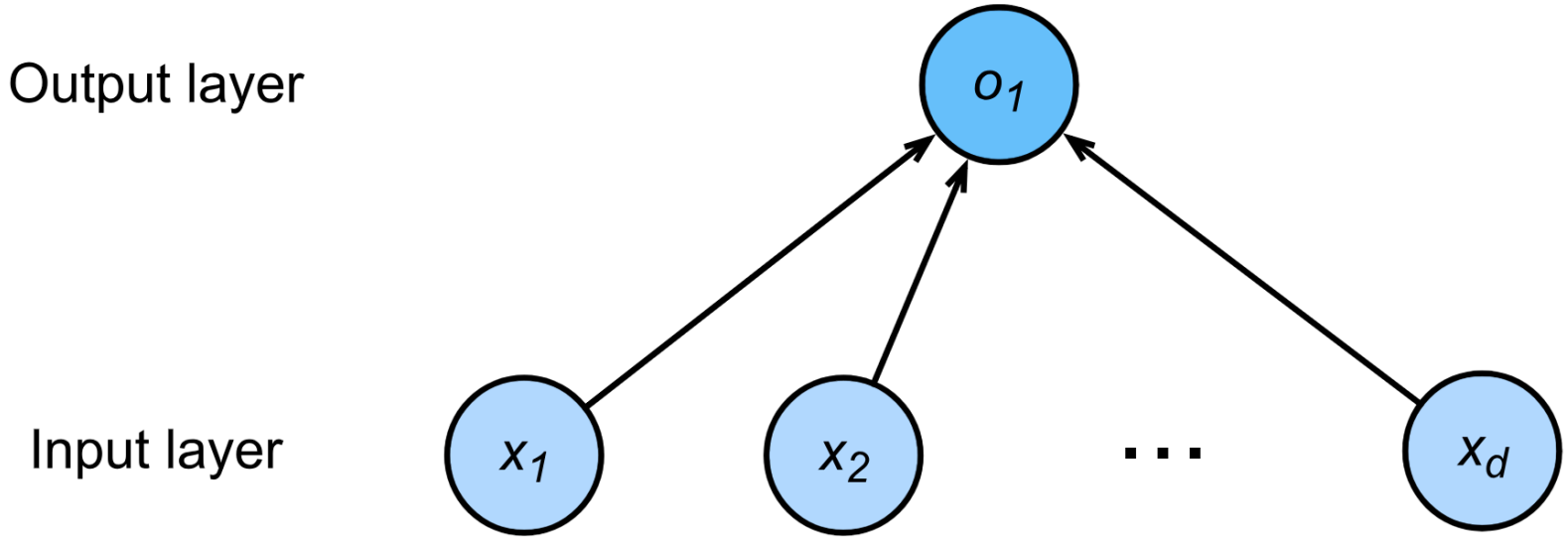
Linear Model as a Single-layer Neural Network



We can stack multiple layers to get deep neural networks

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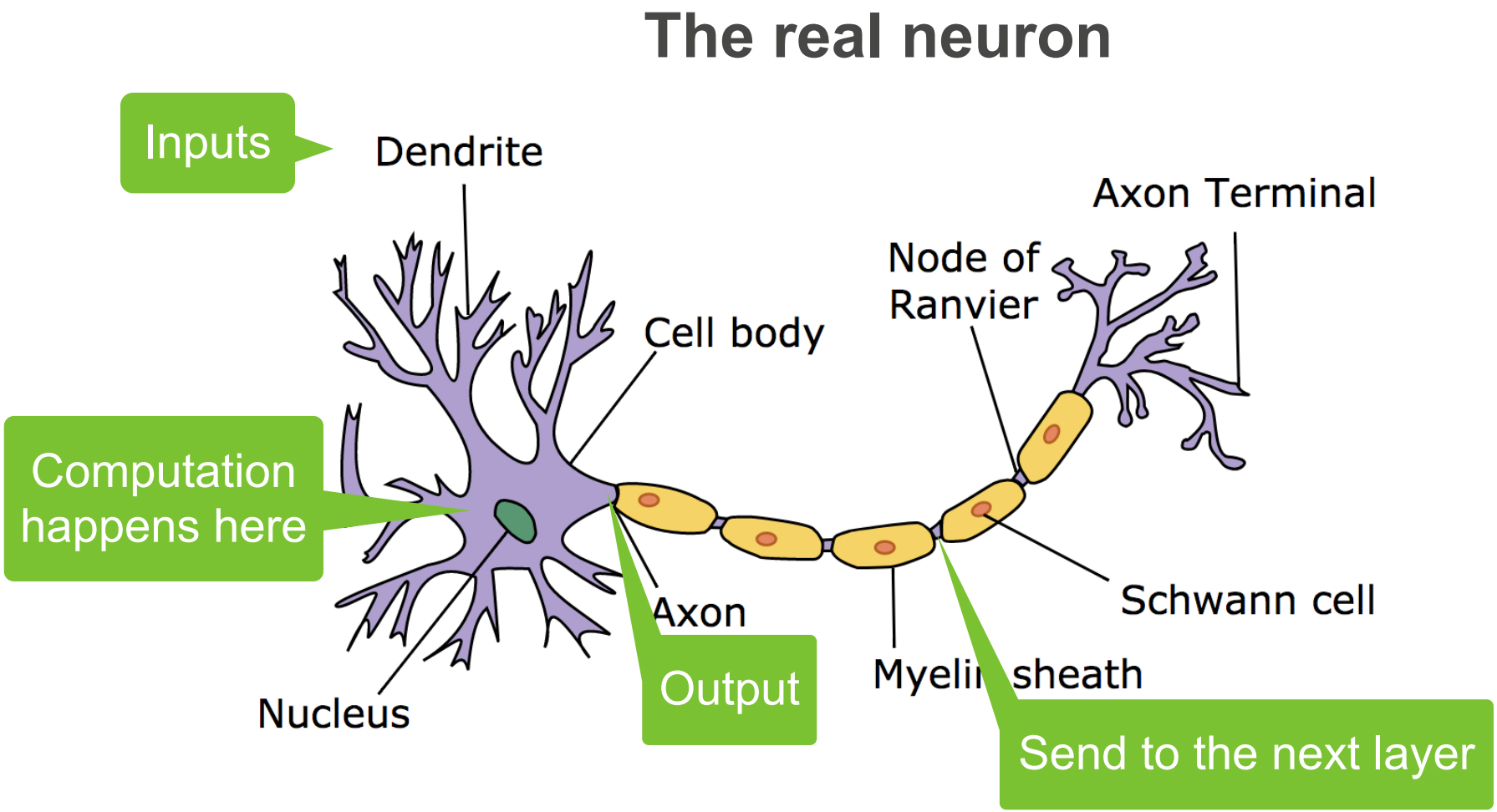
Neural Networks Derive from Neuroscience



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Measure Estimation Quality

- Compare the true value vs the estimated value
  Real sale price vs estimated house price
- Let y the true value, and $\hat{y}$ the estimated value, we can compare the loss

$$\ell(y, \hat{y}) = \left(y - \hat{y}\right)^2$$

  It is called squared loss

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Training Data

- Collect multiple data points to fit parameters
  Houses sold in the last 6 months
- It is called the training data
- The more the better
- Assume *n* examples

$$\mathbf{X} = \left[\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n\right]^T \quad \mathbf{y} = \left[y_0, y_1, \ldots, y_n\right]^T$$

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Learn Parameters

- Training loss

$$\ell(\mathbf{X}, \mathbf{y}, \mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \langle \mathbf{x}_i, \mathbf{w} \rangle - b\right)^2 = \frac{1}{n} \left\| \mathbf{y} - \mathbf{X}\mathbf{w} - b \right\|^2$$

- Minimize loss to learn parameters

$$\mathbf{w}^*, \mathbf{b}^* = \arg\min_{\mathbf{w}, b} \ell(\mathbf{X}, \mathbf{y}, \mathbf{w}, b)$$

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Closed-form Solution

- Add bias into weights by $\mathbf{X} \leftarrow [\mathbf{X}, \mathbf{1}] \quad \mathbf{w} \leftarrow \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}$

$$\ell(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{1}{n} \left\| \mathbf{y} - \mathbf{X}\mathbf{w} \right\|^2 \qquad \frac{\partial}{\partial \mathbf{w}} \ell(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{2}{n} \left(\mathbf{y} - \mathbf{X}\mathbf{w} \right)^T \mathbf{X}$$

- Loss is convex, so the optimal solutions satisfies

$$\frac{\partial}{\partial \mathbf{w}} \ell(\mathbf{X}, \mathbf{y}, \mathbf{w}) = 0$$

$$\Leftrightarrow \frac{2}{n} \left(\mathbf{y} - \mathbf{X}\mathbf{w} \right)^T \mathbf{X} = 0$$

$$\Leftrightarrow \mathbf{w}^* = \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}\mathbf{y}$$

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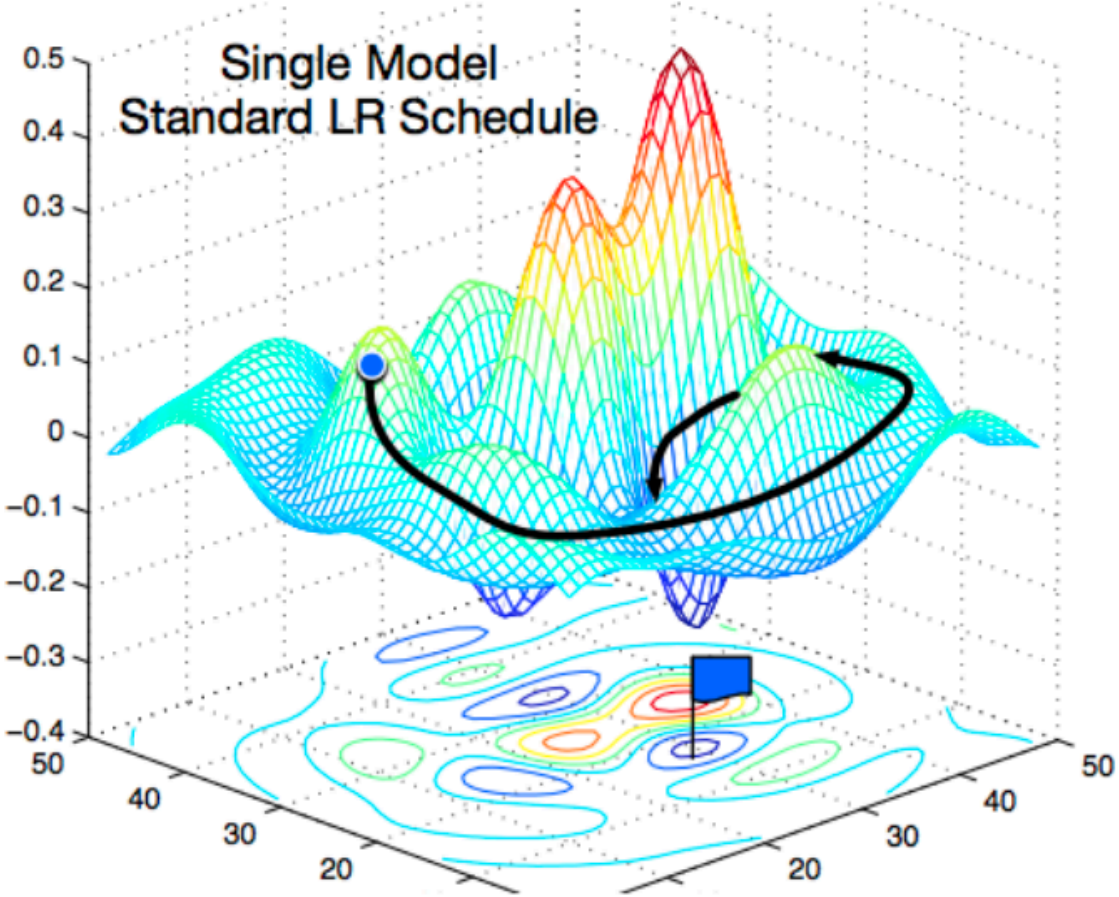
Basic Optimization



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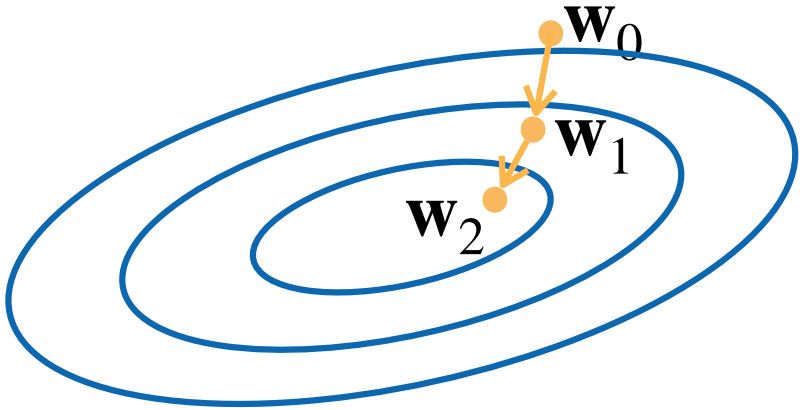
Gradient Descent

- Choose a staring point $\mathbf{w}_0$
- Repeat to update the weight *t=1,2,3*

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \eta \frac{\partial \ell}{\partial \mathbf{w}_{t-1}}$$



  - Gradient: a direction that increases the value
  - Learning rate: a hyper-parameter specifies the step length

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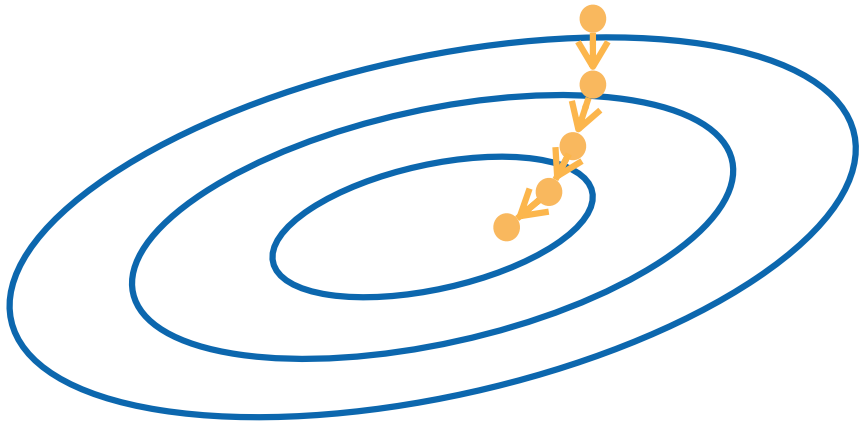
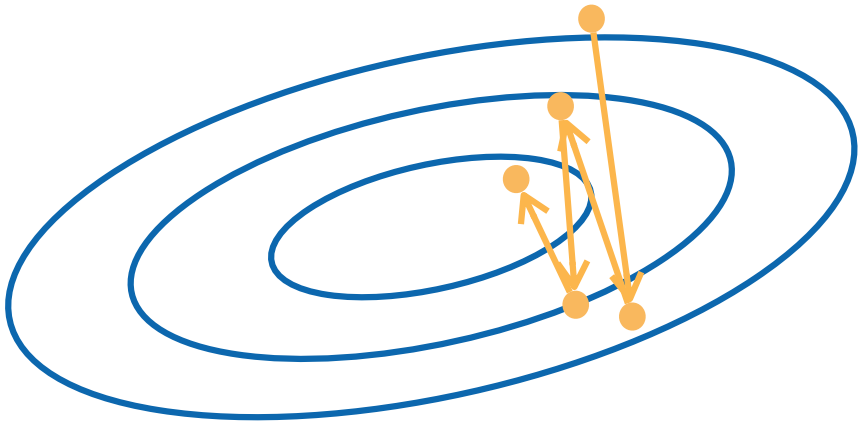
Choose a Learning Rate

Not too small



Not too big



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Mini-batch Stochastic Gradient Descent (SGD)

- Computing the gradient over the whole training data is too expensive
  - Takes minutes to hours for DNN models
- Randomly sample *b* examples $i_1, i_2, \ldots, i_b$ to approximate the loss

$$\frac{1}{b} \sum_{i \in I_b} \ell(\mathbf{x}_i, y_i, \mathbf{w})$$

  - *b* is the batch size, another important hyper-parameters

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Choose a Batch Size

Not too small

Workload is too small, hard to fully utilize computation resources

Not too big

Memory issue
Waste computation, e.g. when all x_i are identical

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Introduction to Deep Learning

5. Maximum Likelihood and Logistic Regression

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Outline

- **Maximum Likelihood**
  - Gauss and means
  - More loss functions (l_1 loss, trimmed mean)
  - Regression revisited
- **Classification**
  - Computing discrete probabilities
  - Likelihood and loss functions
- **Information Theory**

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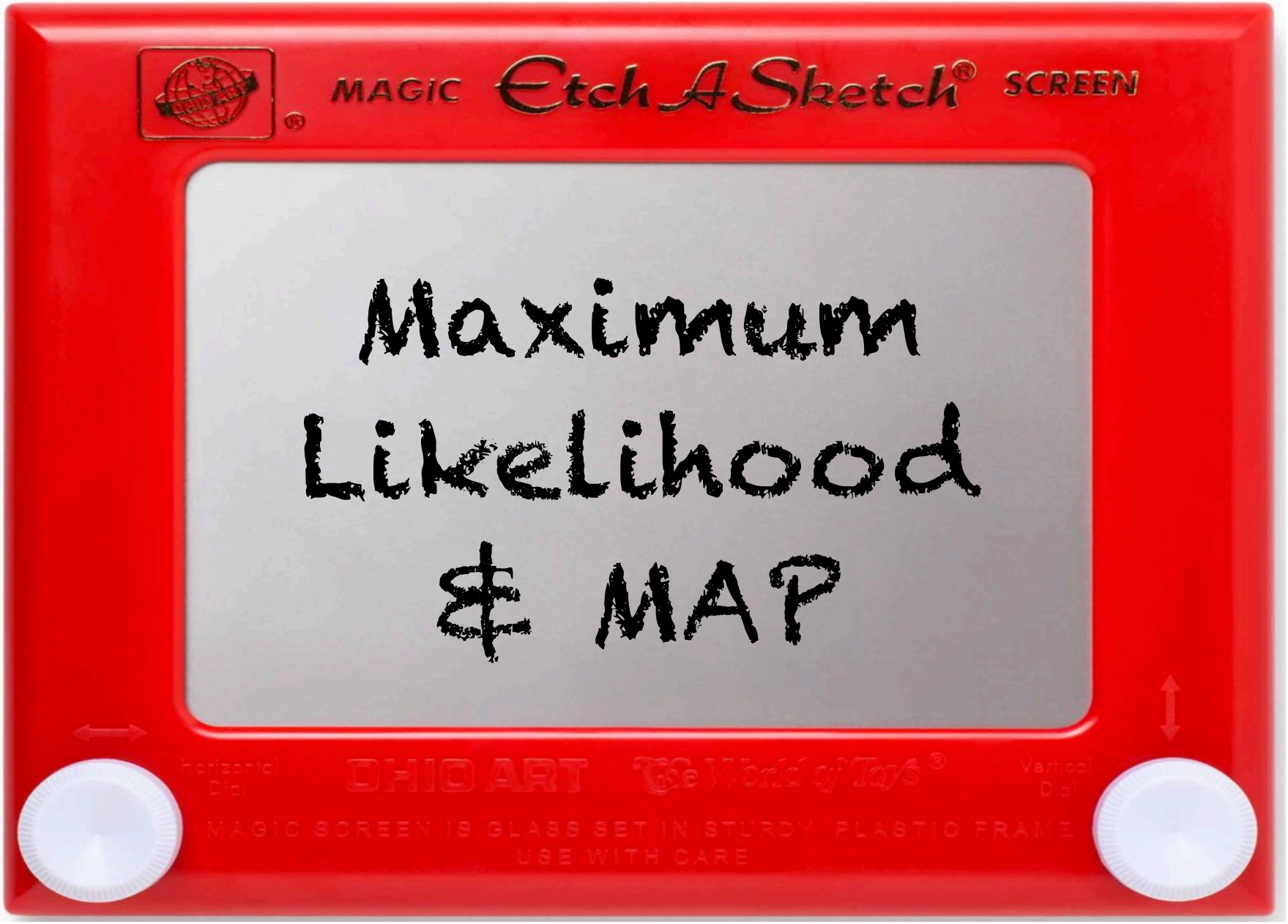
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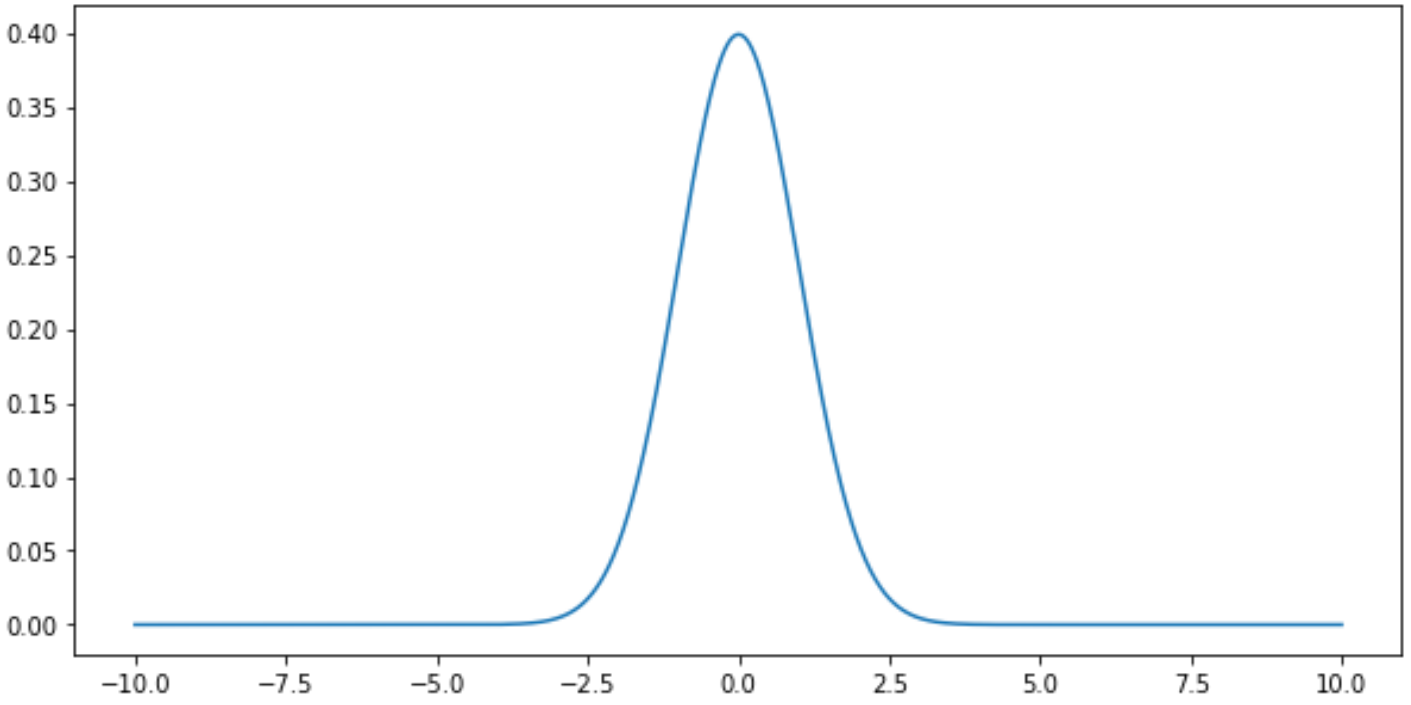
Normal Distribution

Density $$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



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Estimating the parameters in a Gaussian

- **Mean**

$$\mu = \mathbf{E}[x] \text{ hence } \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- **Variance**

$$\sigma^2 = \mathbf{E}\left[(x-\mu)^2\right] \text{ hence } \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n} (x_i - \hat{\mu})^2$$

Why?

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Likelihood

- Observe some data $X = \{x_1, \ldots x_n\}$
- Assume that the data is drawn from a Gaussian

$$p(X; \mu, \sigma^2) = \prod_{i=1}^{n} p(x_i; \mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{2\pi\sigma^2} \exp\left(-\frac{(x_i - \mu)^2}{2\sigma^2}\right)$$

- **Fitting parameters is maximizing** $p(X; \mu, \sigma^2)$ **wrt.** μ, σ^2 (maximize likelihood that data was generated by model)
- **Practical simplification**

$$\underset{\mu,\sigma^2}{\text{maximize}}\, p(X; \mu, \sigma^2) \iff \underset{\mu,\sigma^2}{\text{minimize}} - \log p(X; \mu, \sigma^2)$$

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Maximum Likelihood

- Estimate parameters by finding ones that explain the data

$$\underset{\mu,\sigma^2}{\text{minimize}} \; -\log p(X;\mu,\sigma^2)$$

- **Decompose likelihood**

$$-\log p(X;\mu,\sigma^2) = \sum_{i=1}^{n} \frac{1}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}(x_i-\mu)^2 = \frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

Minimized for $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$

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Maximum Likelihood

- Estimating the variance

$$\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$

- Take derivatives with respect to it

$$\partial_{\sigma^2}[\cdot] = \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\sum_{i=1}^{n}(x_i - \mu)^2 = 0$$

$$\implies \sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

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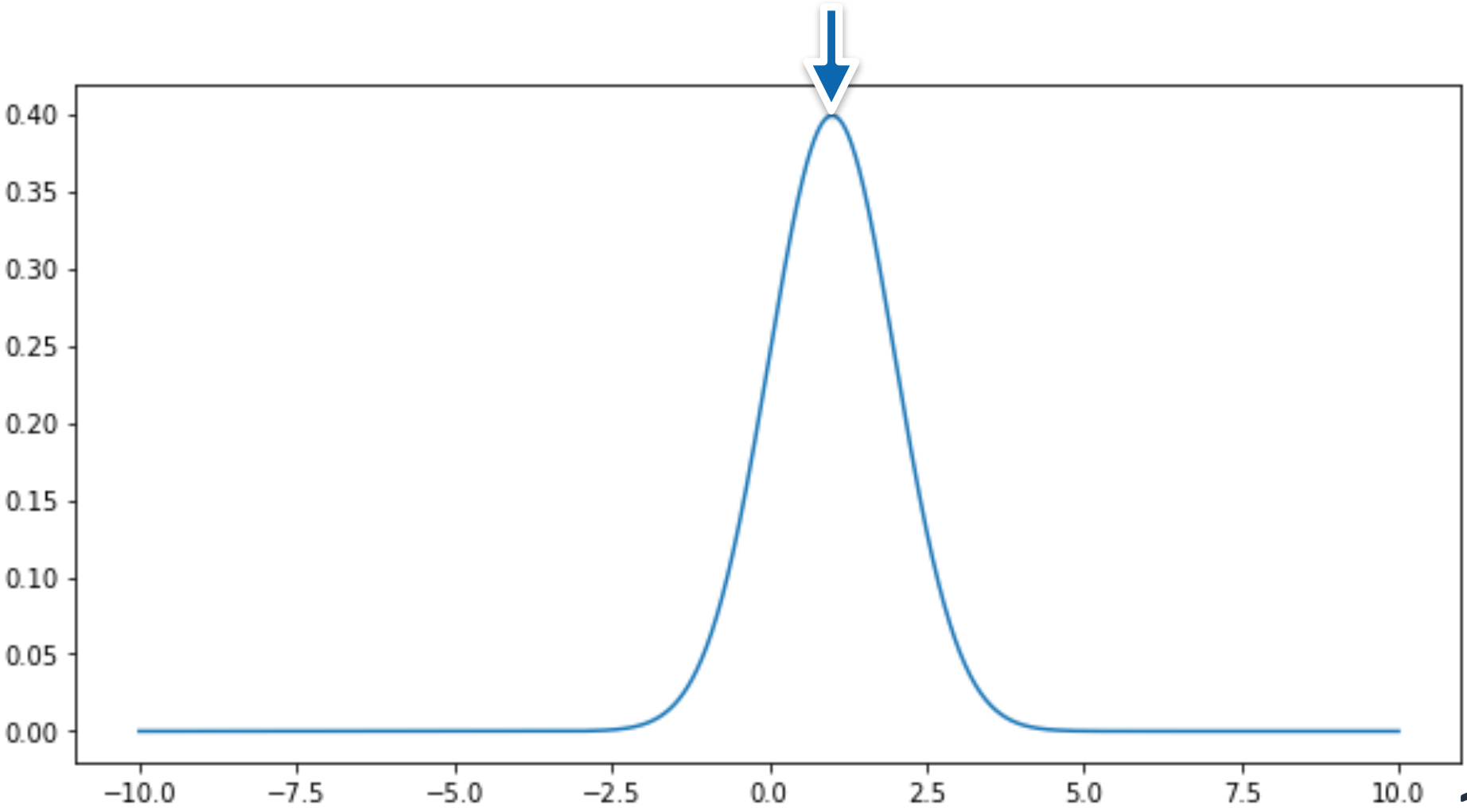
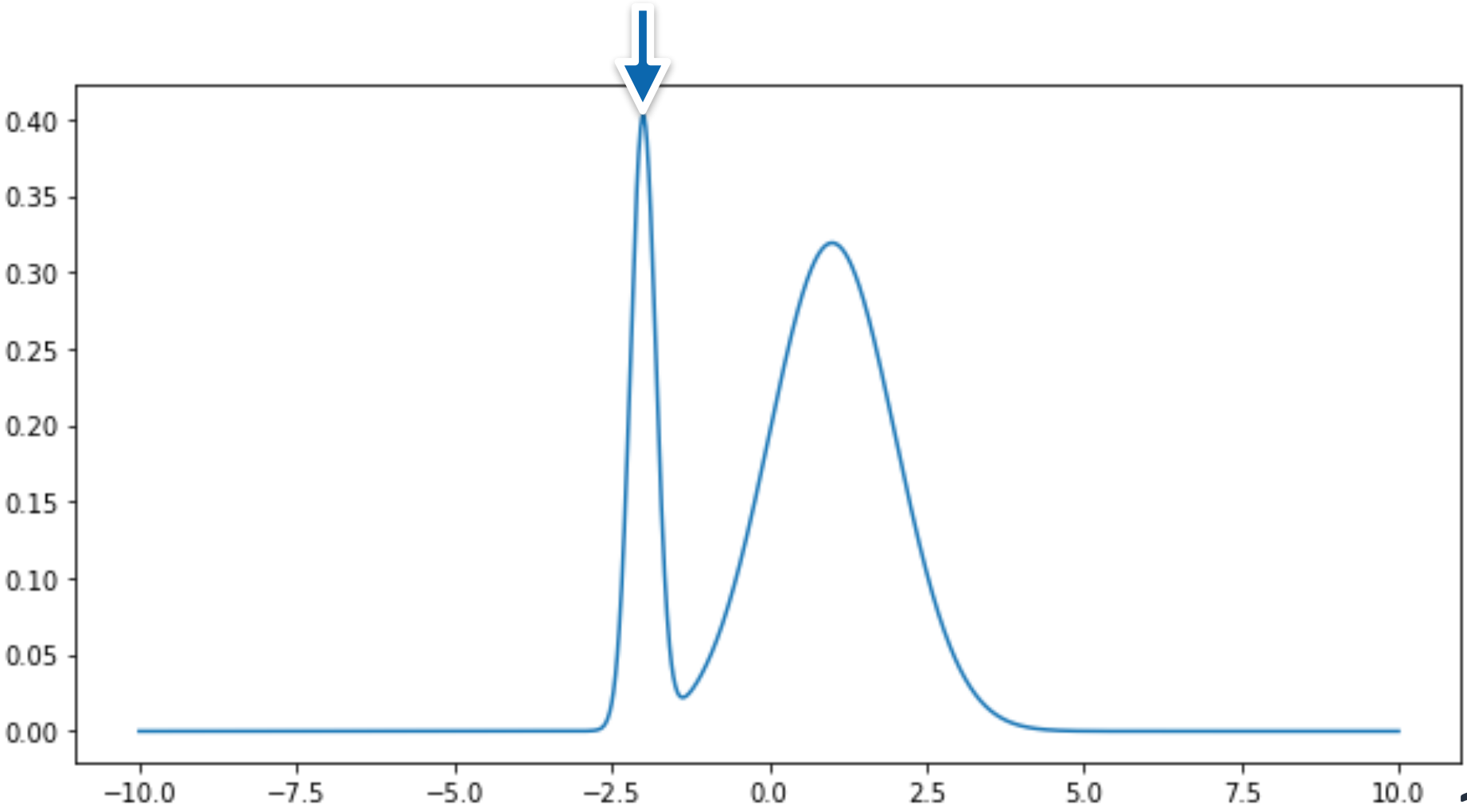
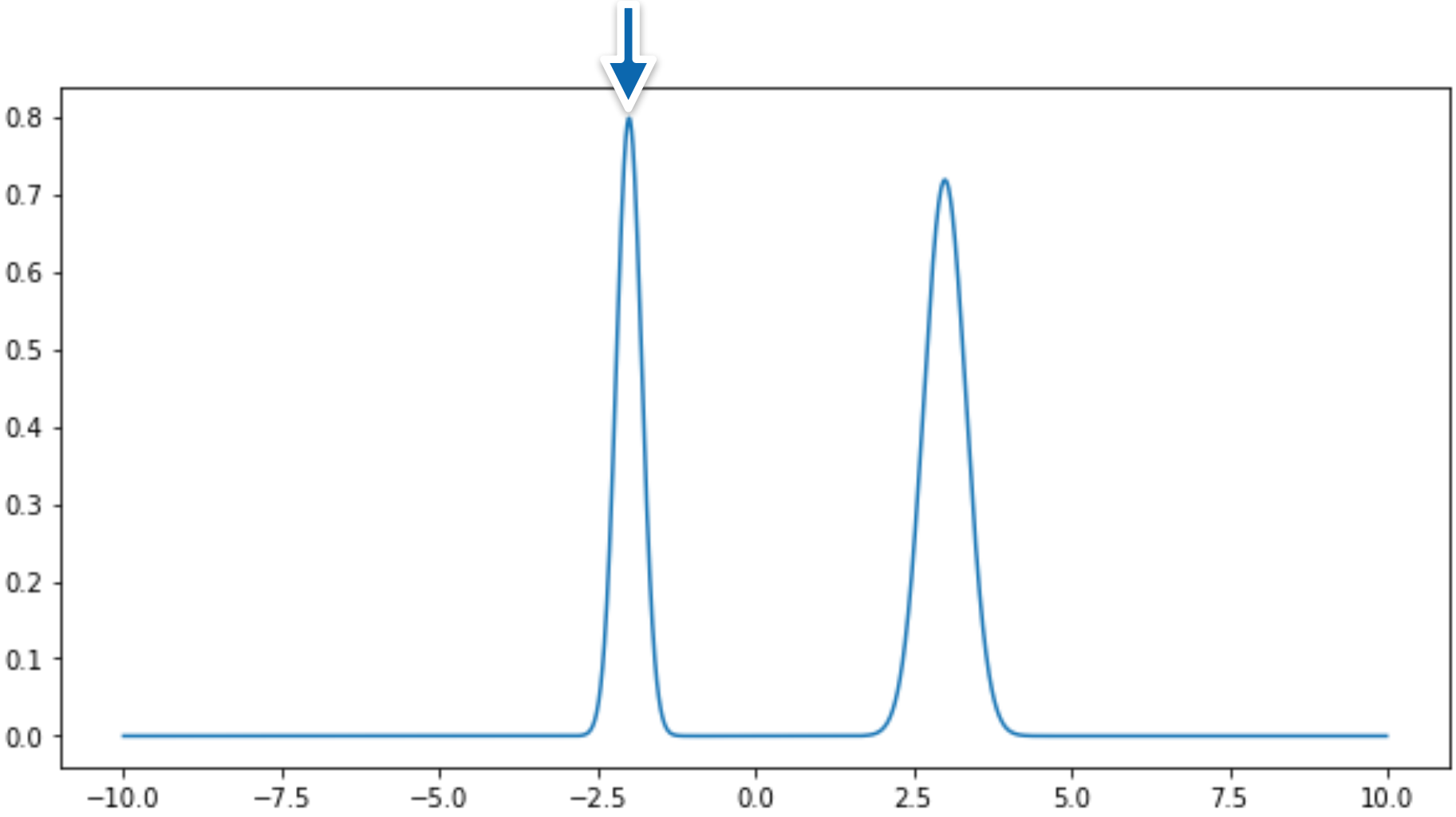
Maximum likelihood estimation



Maximum likelihood estimation



Maximum likelihood estimation



Maximum likelihood estimation

- Data - ‘student didn’t do homework’
- Possible parameters
  - **‘dog ate homework’**
  - **‘abducted by aliens’**
  - **‘too lazy’**
  - **‘sick grandmother’**

Should we believe all?

- **All parameters explain the data.**

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Maximum a posteriori estimation

- Posterior Probability

$$p(w \mid X) \propto p(X \mid w) p(w)$$

penalty

$$\text{hence} \quad -\log p(w \mid X) = -\log p(X \mid w) - \log p(w) + c$$

- Maximum a Posteriori Estimation

$$\underset{w}{\text{minimize}} \; -\log p(X; w) - \log p(w)$$

- No homework example
  p('no homework'|explanation) = 1 (all explanations work)

lazy student	grandma sick	dog ate it	alien abduction
0.8	0.19	0.0099	0.0001

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What does this have to do with regression?

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Regression

- Recall optimization problem

$$\underset{w}{\text{minimize}} \sum_{i=1}^{n} (y_i - f(x_i, w))^2 + \text{penalty}(w)$$

$-\log p(w)$

Does the model work?

Additive Gaussian Noise

- Data generation model

$$y_i = f(x_i, w) + \epsilon_i \text{ where } \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

- Gaussian Prior $p(w)$ hence $-\log p(w) = \frac{1}{2\bar{\sigma}^2}\|w\|^2 + \text{const}.$

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Regression

- Maximum a posteriori

$$\begin{aligned}
&\underset{w}{\text{minimize}} \; -\log p(w \mid X, Y) \\
\iff &\underset{w}{\text{minimize}} \; \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - f(x_i, w))^2 + \frac{1}{2\bar{\sigma}^2} \|w\|^2 + \text{const}. \\
\iff &\underset{w}{\text{minimize}} \; \frac{1}{2n} \sum_{i=1}^{n} (y_i - f(x_i, w))^2 + \frac{\lambda}{2} \|w\|^2
\end{aligned}$$

Implement this

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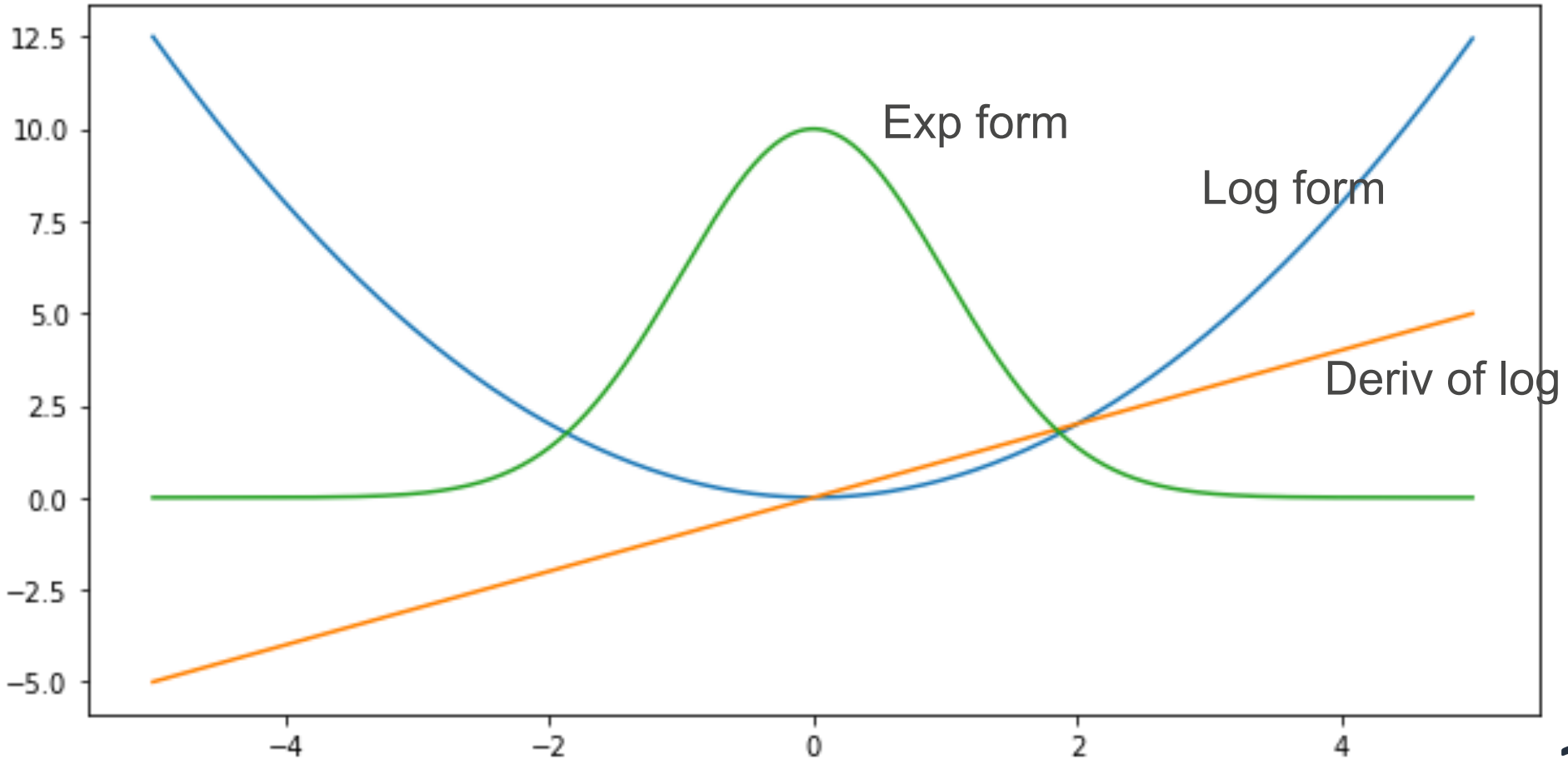
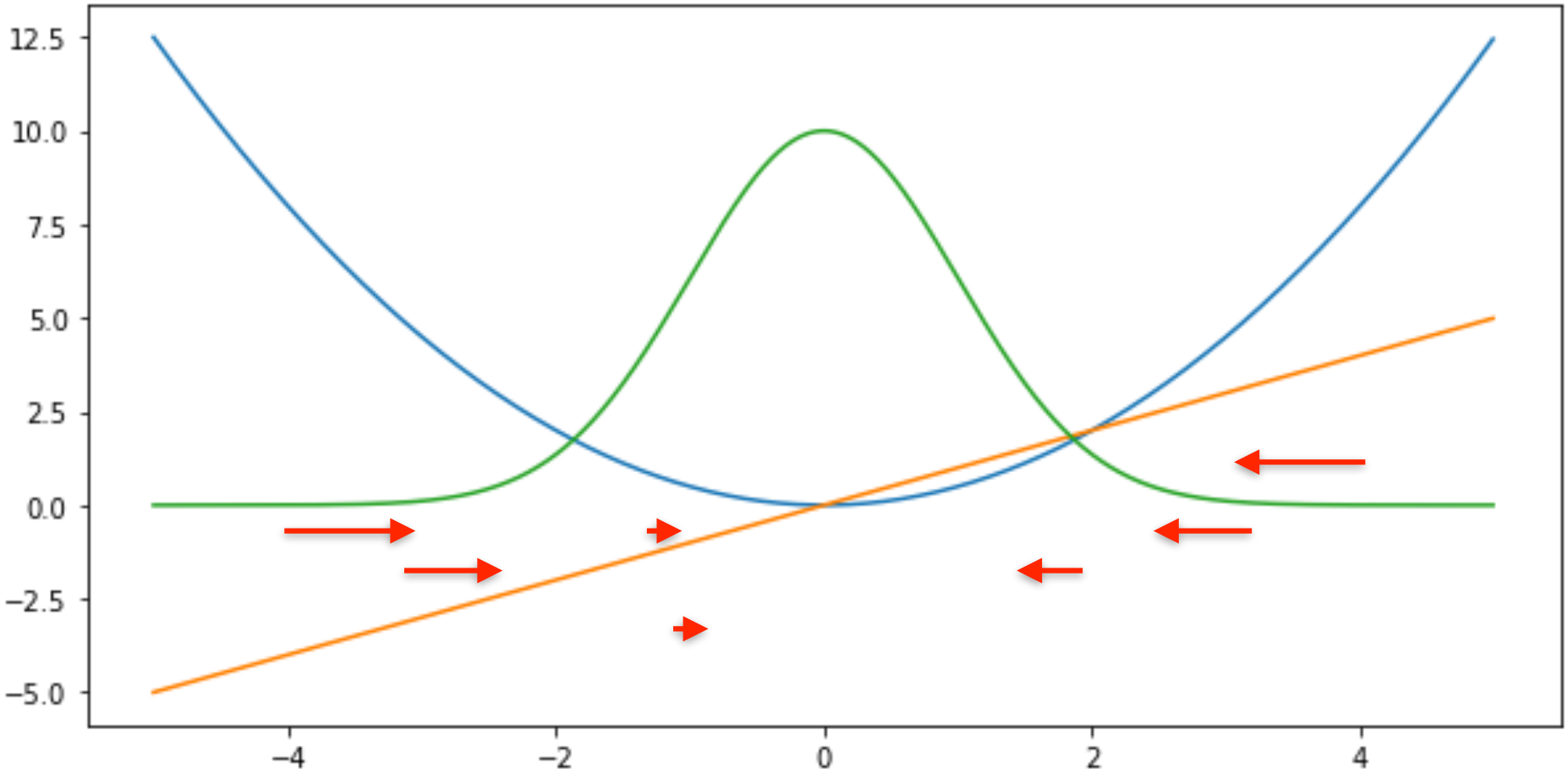
L2 Loss

$$l(y, y') = \frac{1}{2}(y - y')^2$$



L2 Loss - mean

$$l(y, y') = \frac{1}{2}(y - y')^2$$



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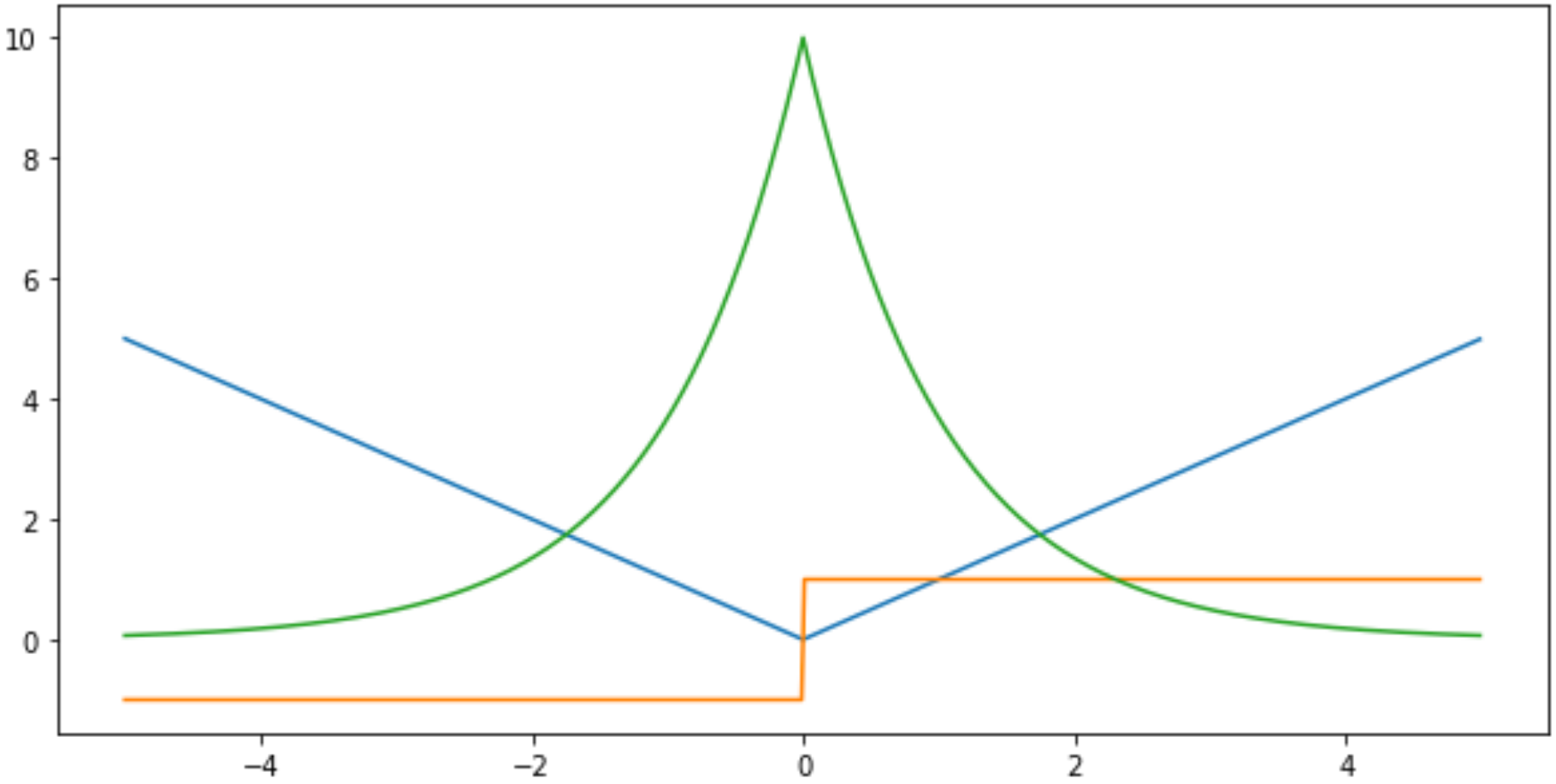
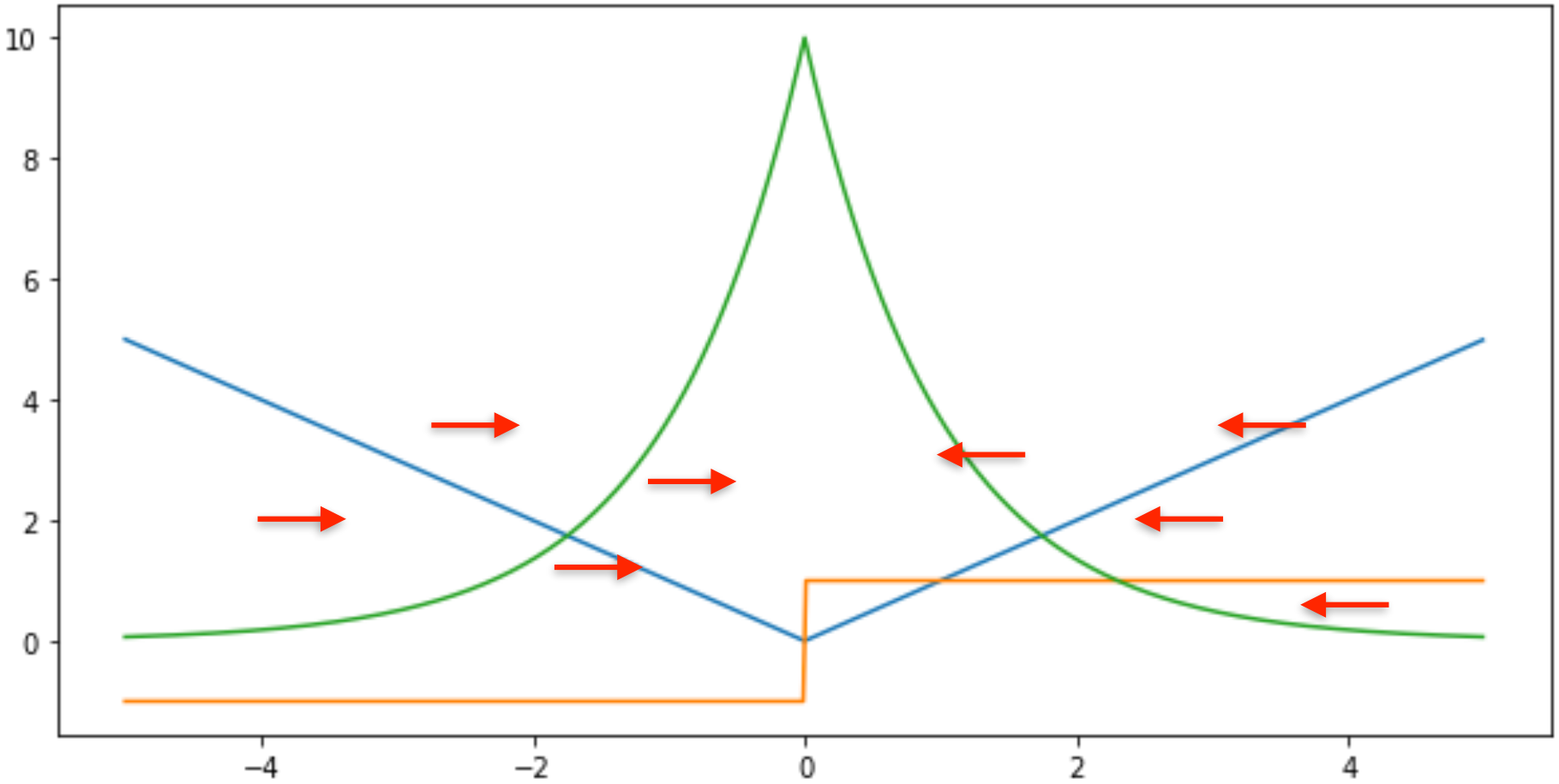
L1 Loss

$$l(y, y') = |y - y'|$$

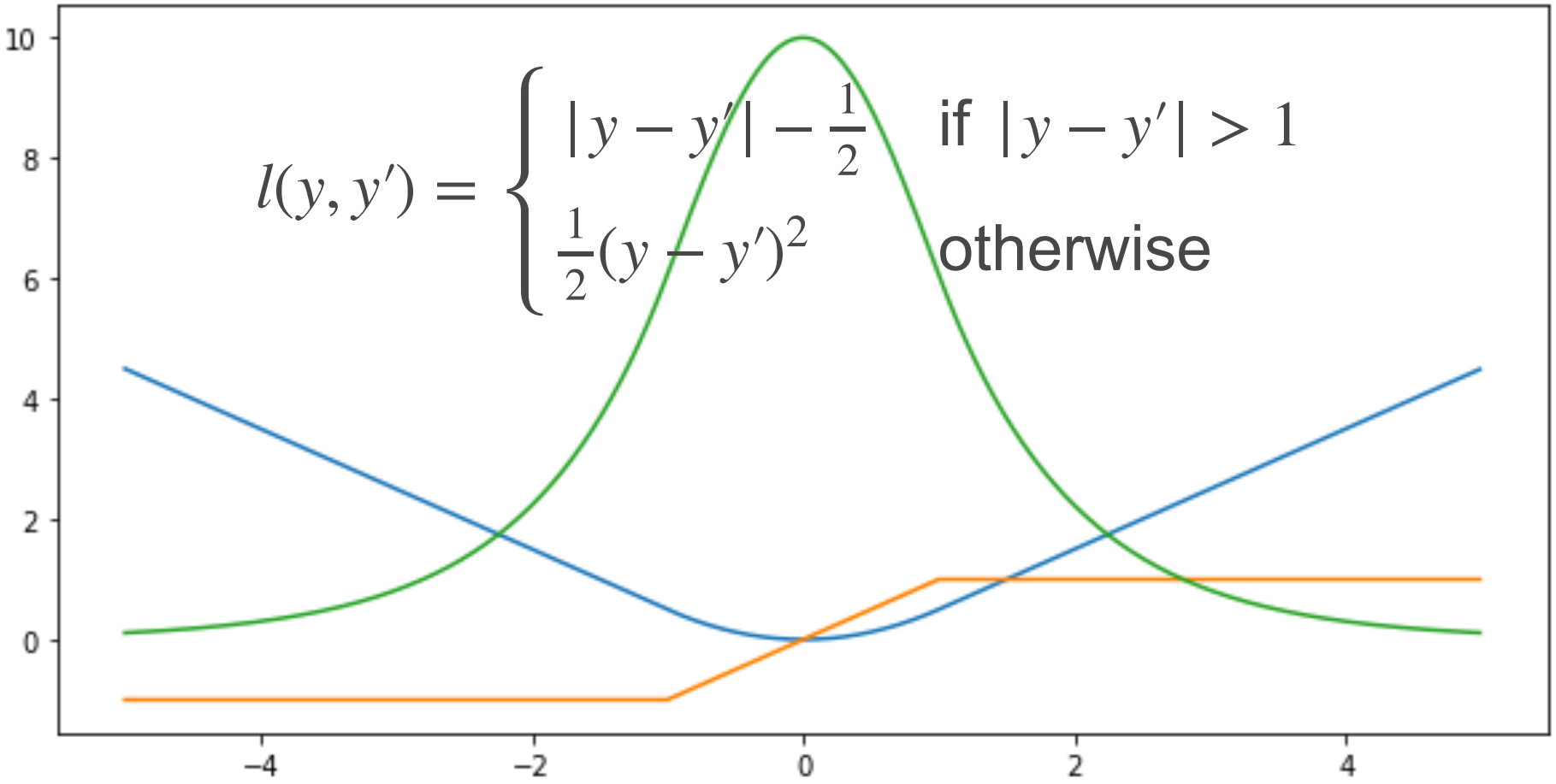


L1 Loss - median $l(y, y') = |y - y'|$

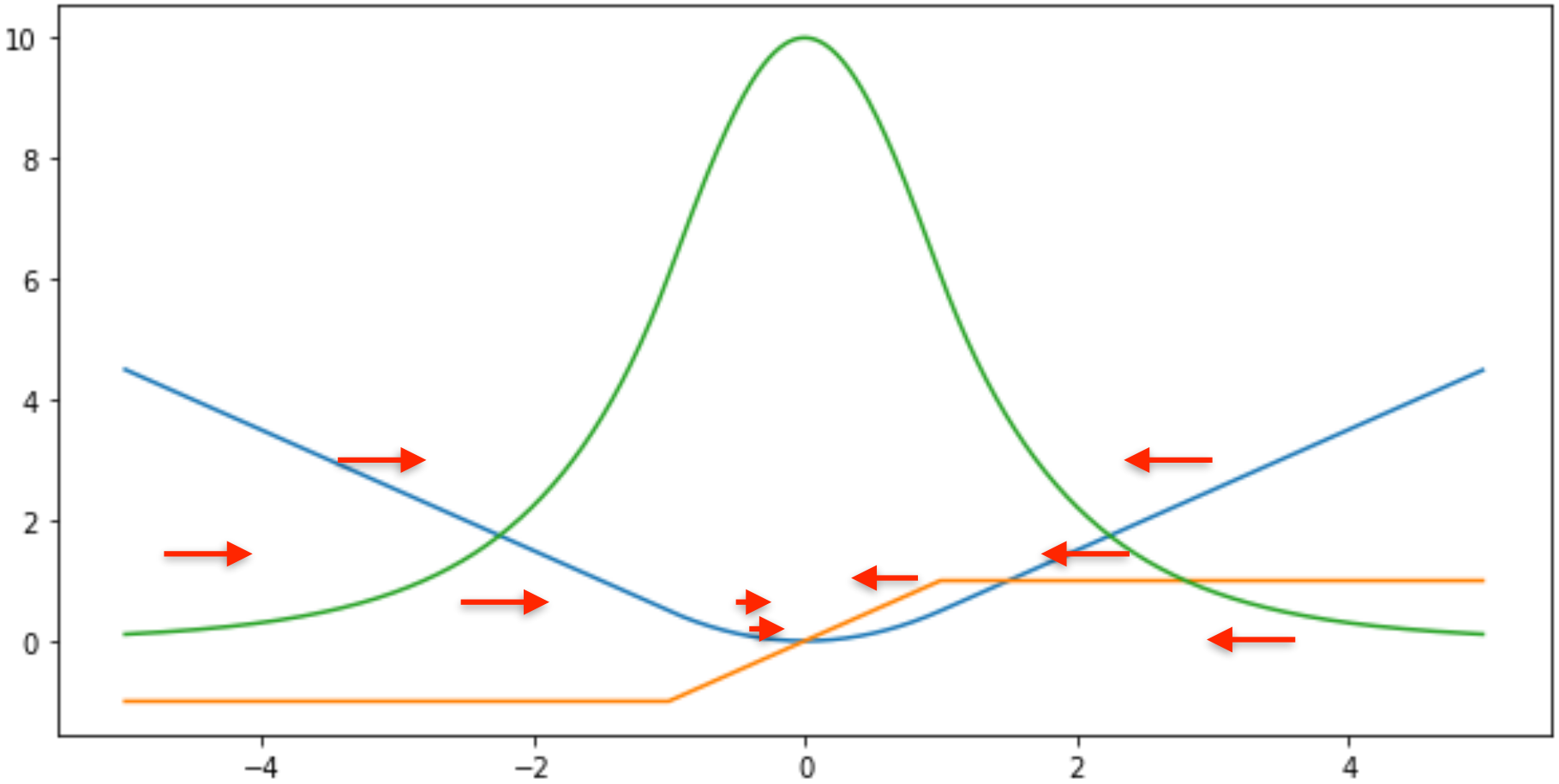


Huber's Robust Loss

$$l(y, y') = \begin{cases} |y - y'| - \frac{1}{2} & \text{if } |y - y'| > 1 \\ \frac{1}{2}(y - y')^2 & \text{otherwise} \end{cases}$$



Huber's Robust Loss - trimmed mean

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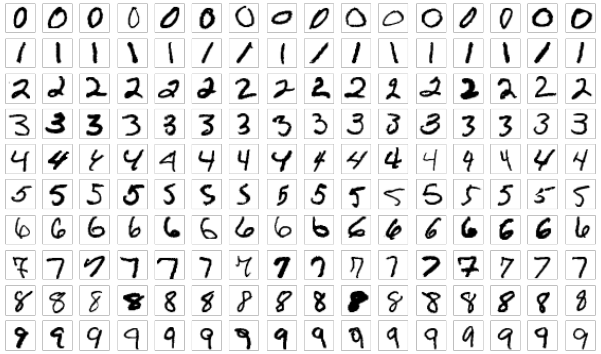
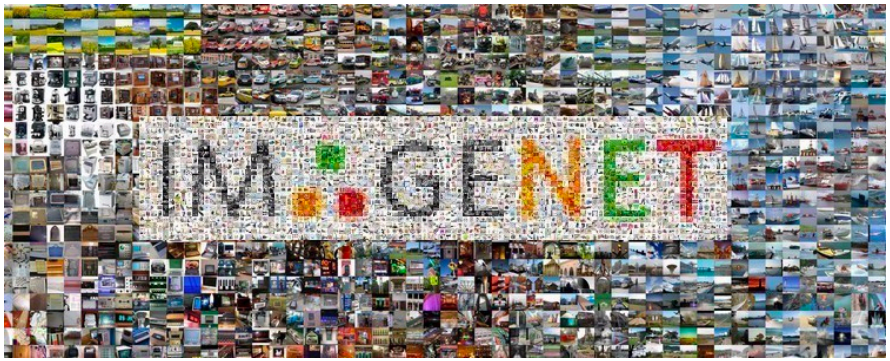
Regression vs. Classification

- Regression estimates a continuous value
- Classification predicts a discrete category

MNIST: classify hand-written digits (10 classes)



ImageNet: classify nature objects (1000 classes)



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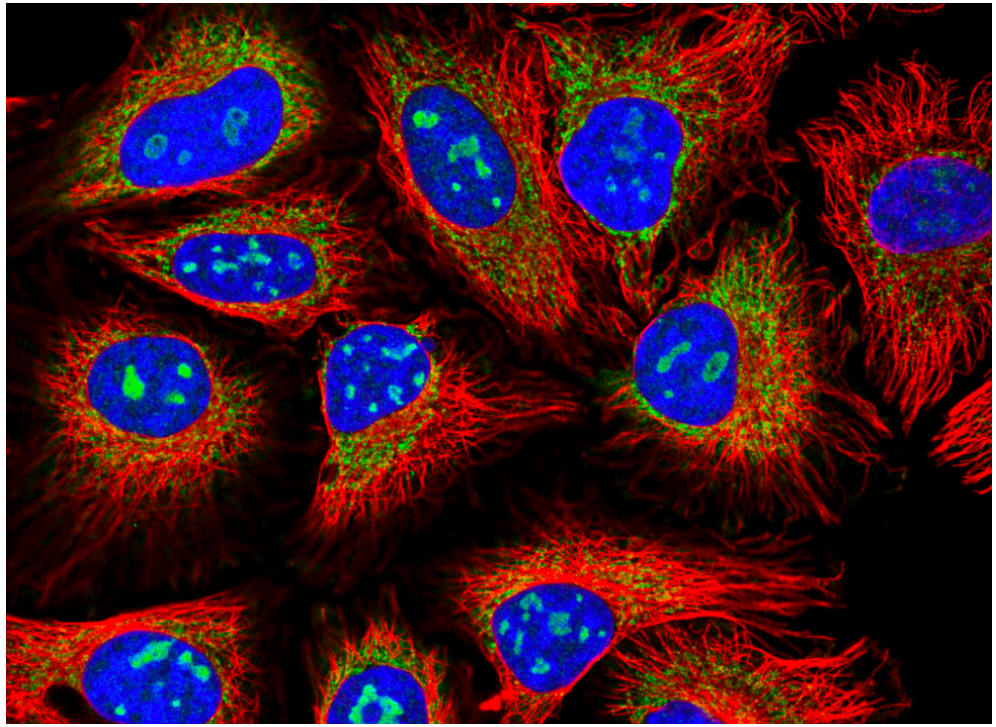
Classification Tasks at Kaggle

Classify human protein microscope images into 28 categories



```
0.  Nucleoplasm
1.  Nuclear membrane
2.  Nucleoli
3.  Nucleoli fibrillar
4.  Nuclear speckles
5.  Nuclear bodies
6.  Endoplasmic reticu
7.  Golgi apparatus
8.  Peroxisomes
9.  Endosomes
10.  Lysosomes
11.  Intermediate fila
12.  Actin filaments
13.  Focal adhesion si
14.  Microtubules
15.  Microtubule ends
16.  Cytokinetic bridg
```

https://www.kaggle.com/c/human-protein-atlas-image-classification

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Classification Tasks at Kaggle

Classify malware into 9 categories

https://www.kaggle.com/c/malware-classification

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Classification Tasks at Kaggle

Classify toxic Wikipedia comments into 7 categories

comment_text	toxic	severe_toxic	obsc
Explanation\nWhy the edits made under my usern...	0	0	0
D'aww! He matches this background colour I'm s...	0	0	0
Hey man, I'm really not trying to edit war. It...	0	0	0
"\nMore\nI can't make any real suggestions on ...	0	0	0
You, sir, are my hero. Any chance you remember...	0	0	0

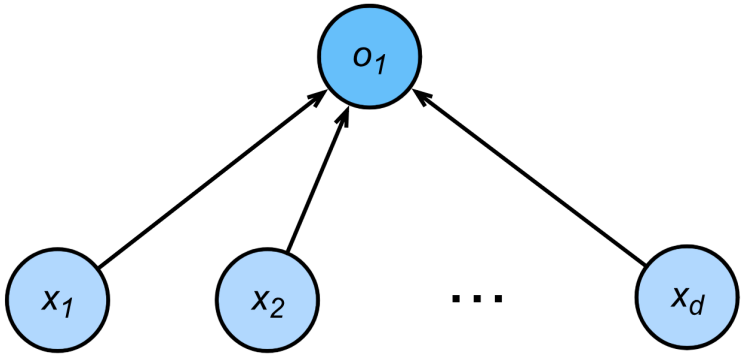
https://www.kaggle.com/c/jigsaw-toxic-comment-classification-challenge

slides adapted from courses.d2l.ai/berkeley-stat-157

From Regression to Multi-class Classification

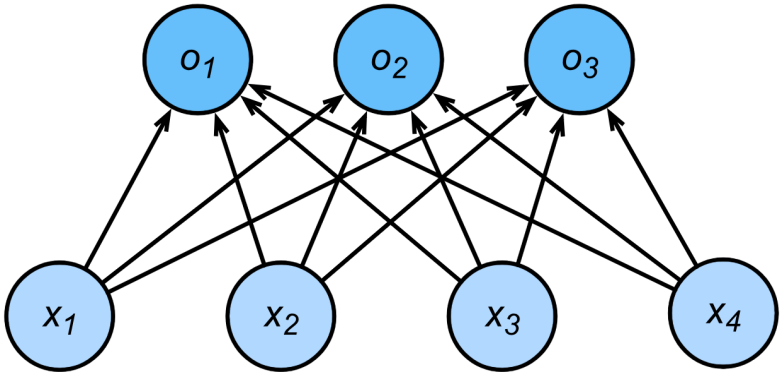
Regression

- Single continuous output
- Natural scale in $\mathbb{R}$
- Loss given e.g. in terms of difference $y - f(x)$



Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



slides adapted from courses.d2l.ai/berkeley-stat-157

From Regression to Multi-class Classification

Square Loss

- One hot encoding per class

$$\mathbf{y} = [y_1, y_2, \ldots, y_n]^\top$$

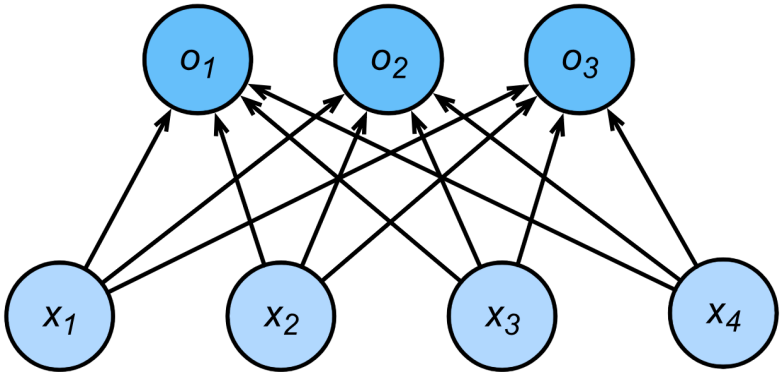
$$y_i = \begin{cases} 1 \text{ if } i = y \\ 0 \text{ otherwise} \end{cases}$$

- Train with squared loss
- Largest output wins

$$\hat{y} = \underset{i}{\operatorname{argmax}}\, o_i$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



slides adapted from courses.d2l.ai/berkeley-stat-157

From Regression to Multi-class Classification

Uncalibrated Scale

- One output per class
- Largest output wins

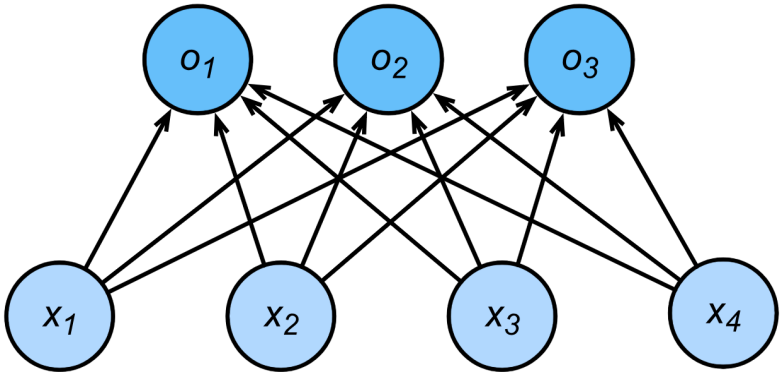
$$\hat{y} = \operatorname*{argmax}_i o_i$$

- Want that correct class is recognized confidently (**large margin**)

$$o_y - o_i \geq \Delta(y, i)$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



slides adapted from courses.d2l.ai/berkeley-stat-157

From Regression to Multi-class Classification

Calibrated Scale

- Output matches probabilities (nonnegative, sums to 1)

$$p(y \mid o) = \text{softmax}(o)$$

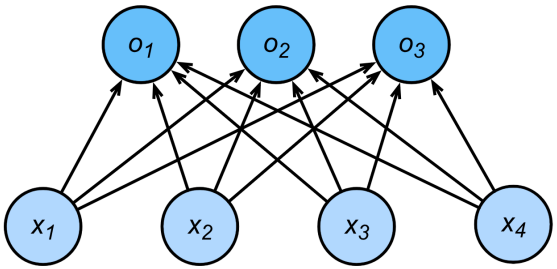
$$= \frac{\exp(o_y)}{\sum_i \exp(o_i)}$$

- Negative log-likelihood

$$-\log p(y \mid y) = \log \sum_i \exp(o_i) - o_y$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



slides adapted from courses.d2l.ai/berkeley-stat-157

Summary

- **Maximum Likelihood**
  - Gauss and means
  - More loss functions (l_1 loss, trimmed mean)
  - Regression revisited
- **Classification**
  - Computing discrete probabilities
  - Likelihood and loss functions

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