Machine Learning

Regression & Gradient Descent

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Recall: Terminology

- Data
  - Data set, feature, dimentionality, label, sample…
- Train & Test
- Task
  - By prediction target
  - By label

Recall: Error and Overfitting

- Error rate/Accuracy
  - $E = \frac{the\ number\ of\ misclassified\ samples\ (a)}{the\ number\ of\ all\ samples\ (m)} = \frac{a}{m}$
- Error
  - Train/Test/Generalization error
- Overfitting
  - Small loss on training data, large loss on testing data
  - Can’t be avoided completely

Recall: Evaluation Methods

- Hold-out
- Cross Validation
- Bootstrapping

Recall: Performance Measure

MSE for Regression $$E(f;D)=\frac{1}{m}\sum_{i=1}^{m}\left(f\left(\boldsymbol{x}_i\right)-y_i\right)^2$$

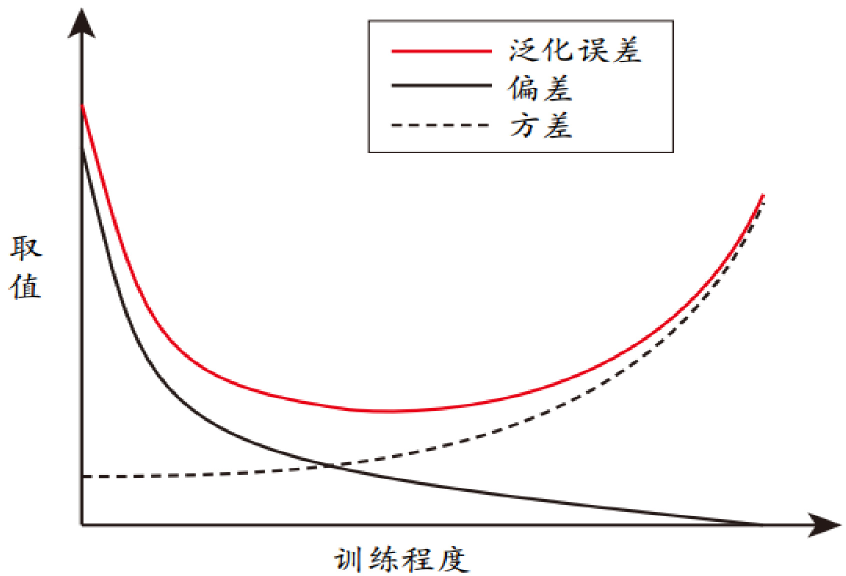
Accuracy for Classification $$\begin{aligned}\operatorname{acc}(f;D) &= \frac{1}{m}\sum_{i=1}^{m}\mathbb{I}\left(f\left(\boldsymbol{x}_i\right)=y_i\right) \\ &= 1-E(f;D)\ .\end{aligned}$$

Precision $P=\dfrac{TP}{TP+FP}$

Recall $R=\dfrac{TP}{TP+FN}$

$$F1=\frac{2*P*R}{P+R}=\frac{2*TP}{the\ number\ of\ samples+TP-TN}$$

Recall: Bias and variance



泛化误差与偏差、方差的关系示意图

Large bias	Large variance
Add more features as input	More data
A more complex model	Regularization

Today's Topics

- Regression
- Linear Regression
- Gradient Descent
- Regularization

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- ***Regression***
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- Gradient Descent
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Different types of functions

Regression: The function outputs a scalar.

Predict PM2.5

PM2.5 today
temperature
Concentration of O_3

f

PM2.5 of tomorrow

Classification: Given options (**classes**), the function outputs the correct one.

Spam filtering

f

Yes/No

Structured Learning

create something with structure (image, document)

Regression, Classification

"man in black shirt is playing guitar."

"construction worker in orange safety vest is working on road."

"two young girls are playing with lego toy."

"boy is doing backflip on wakeboard."

"girl in pink dress is jumping in air."

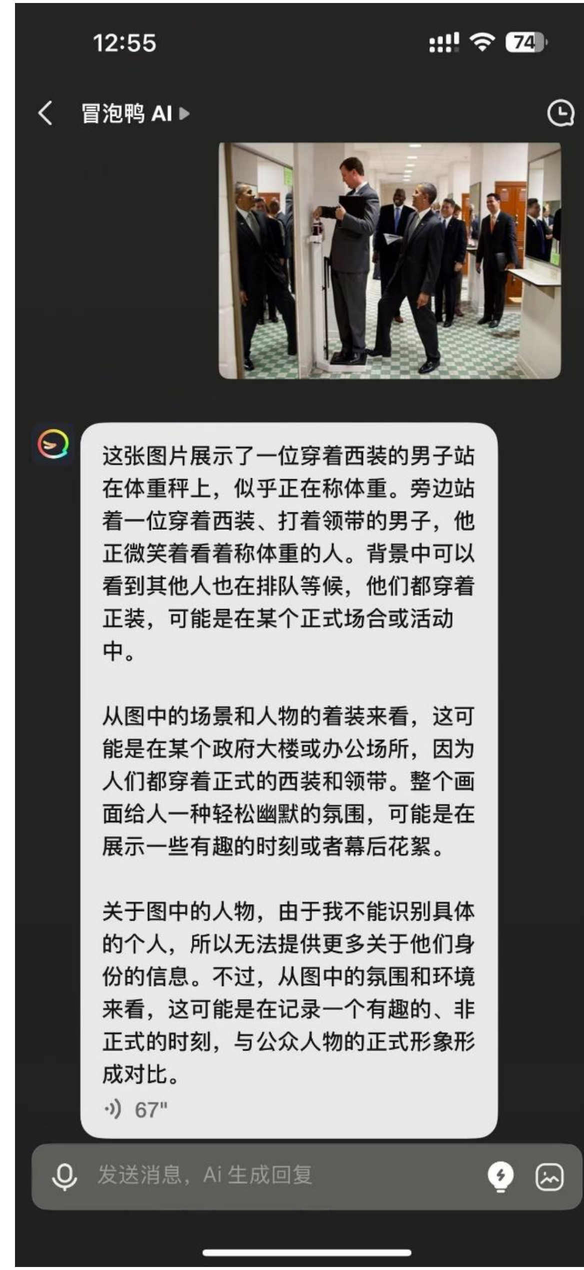
"black and white dog jumps over bar."

"young girl in pink shirt is swinging on swing."

"man in blue wetsuit is surfing on wave."


12:52
新对话
doubao.com
AI 编辑
图中人物有美国前总统奥巴马。画面展现的是在一个类似更衣室或准备区域的走廊场景，周围还有多位身着正装的人士 。这可能是某次活动前的准备场景。奥巴马曾是美国第 44 任总统，在任期间推行了一系列如医保改革等政策。
拍题答疑
AI 生图
照片动起来
打电话
发消息...


12:53
Kimi
问 kimi.com，做 PPT，写作更方便。
描述一下图片内容
Kimi
这张图片显示了一群人在一个室内环境中。前景中，一位穿着西装的男士正在使用一个身高测量仪测量自己的身高，他站在一个白色的测量台上。旁边站着另一位穿着西装的男士，手里拿着文件，似乎在观察测量过程。背景中还有其他几位穿着正式服装的男士，他们站在走廊里，似乎在等待或观察。整个场景看起来像是在一个正式的场合，可能是一个政府大楼或类似的机构。
拍照解题
打电话
图片创作
翻译
有什么问题尽管问我


12:55
冒泡鸭 AI
这张图片展示了一位穿着西装的男子站在体重秤上，似乎正在称体重。旁边站着一位穿着西装、打着领带的男子，他正微笑着看着称体重的人。背景中可以看到其他人也在排队等候，他们都穿着正装，可能是在某个正式场合或活动中。
从图中的场景和人物的着装来看，这可能是在某个政府大楼或办公场所，因为人们都穿着正式的西装和领带。整个画面给人一种轻松幽默的氛围，可能是在展示一些有趣的时刻或者幕后花絮。
关于图中的人物，由于我不能识别具体的个人，所以无法提供更多关于他们身份的信息。不过，从图中的氛围和环境来看，这可能是在记录一个有趣的、非正式的时刻，与公众人物的正式形象形成对比。
67"
发送消息，AI 生成回复

Regression

- Stock Market Forecast

$f($  $) =$ Dow Jones Industrial Average at tomorrow

- Self-driving Car

$f($  $) =$ 方向盘角度

- Recommendation

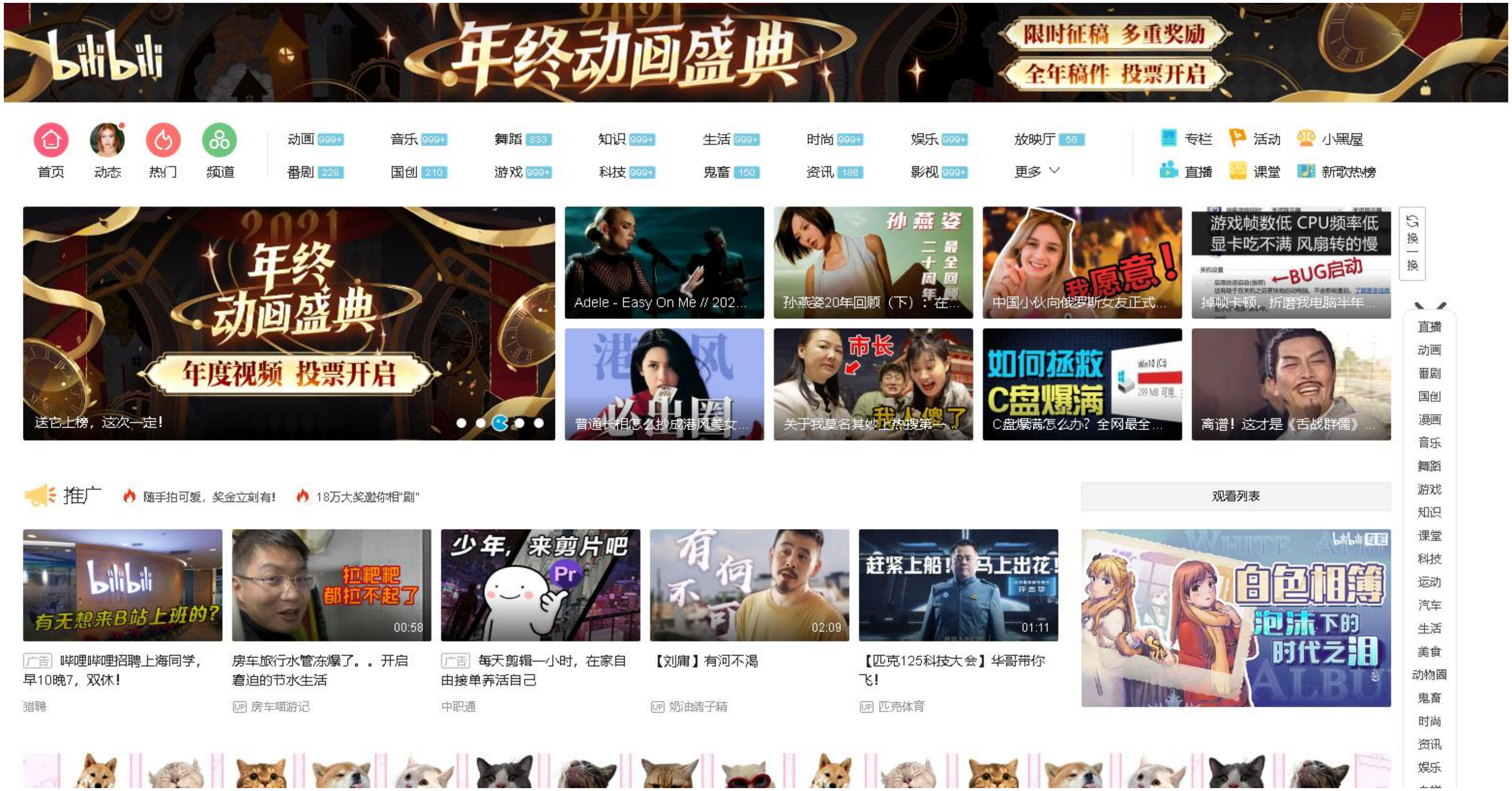
$f($ User A Commodity B $) =$ 购买可能性

Today's Topics

- Regression
- ***Linear Regression***
- Gradient Descent
- Regularization

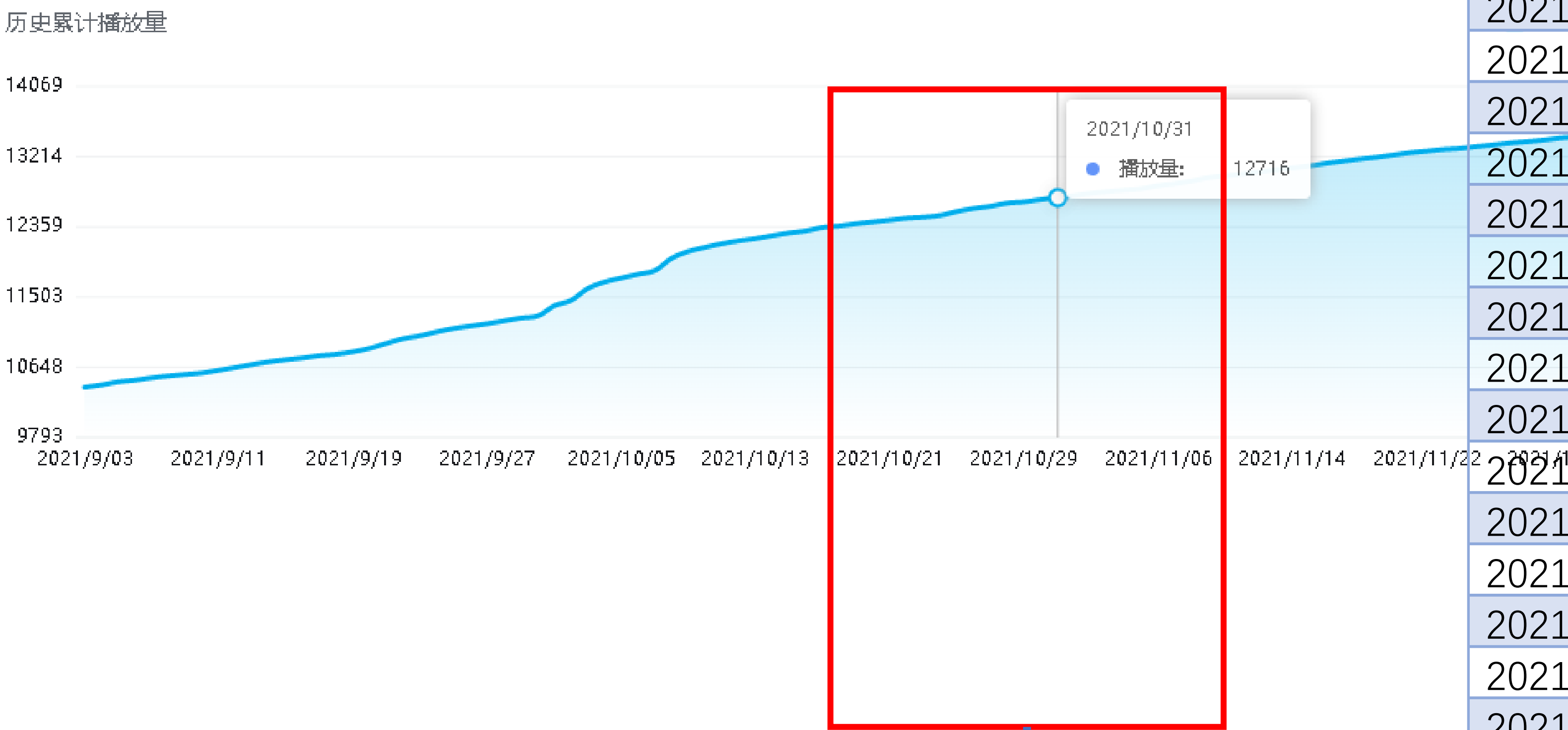
How to find a good function?

- **A bilibili case study**



How to find a good function?

- **A bilibili case study**



时间	播放量
2021-10-21	12442
2021-10-22	12465
2021-10-23	12478
2021-10-24	12499
2021-10-25	12547
2021-10-26	12584
2021-10-27	12610
2021-10-28	12648
2021-10-29	12664
2021-10-30	12692
2021-10-31	12716
2021-11-01	12740
2021-11-02	12769
2021-11-03	12790
2021-11-04	12808
2021-11-05	12825
2021-11-06	12863

The function we want to find …

$$y = f\Big($$

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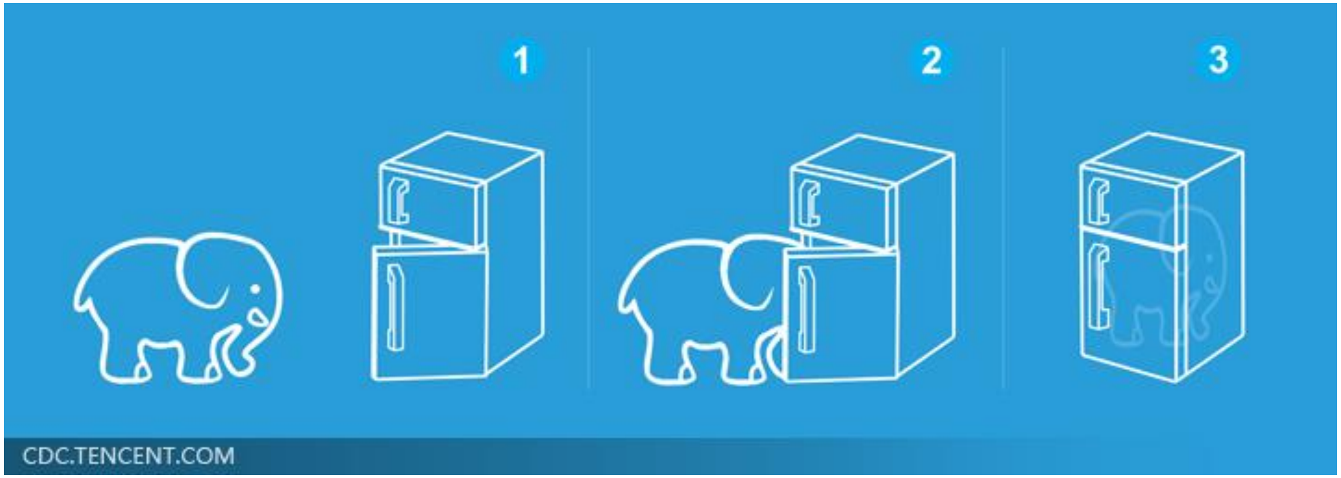
$$\Big)$$

no. of views
on 11/18

Typical process of ML

Step 1: function with unknown param → Step 2: define loss from training data → Step 3: optimization



Step1: Function with Unknown Parameters

$$y = f(\quad)$$

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Model $y = b + wx_1$ based on domain knowledge

feature

y: no. of views on 11/18, x_1: no. of views on 11/17

w and b are unknown parameters (learned from data)

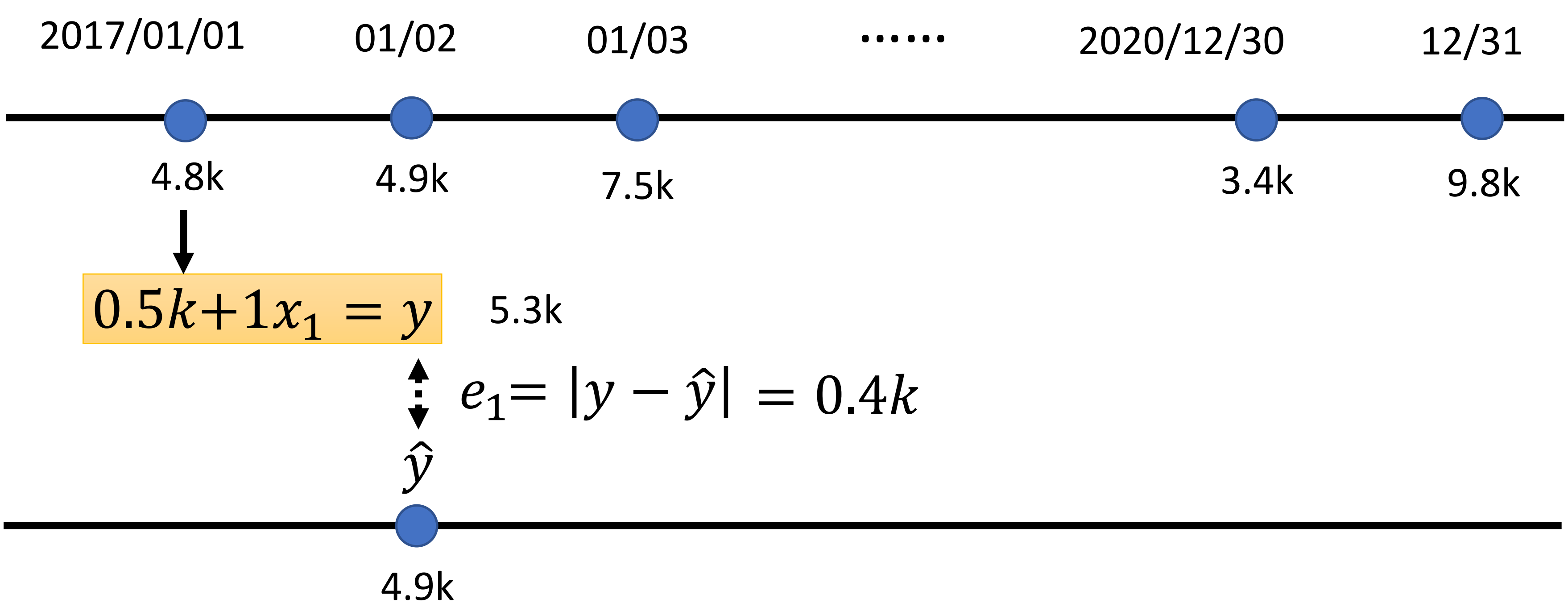
weight **bias**

Step2: Define Loss from Training Data

- ➢ Loss is a function of parameters $L(b, w)$
- ➢ Loss: how good a set of values is.

$L(0.5k, 1)$ $\quad y = b + wx_1 \longrightarrow y = 0.5k + 1x_1$ How good it is?

Data from 2017/01/01 – 2020/12/31



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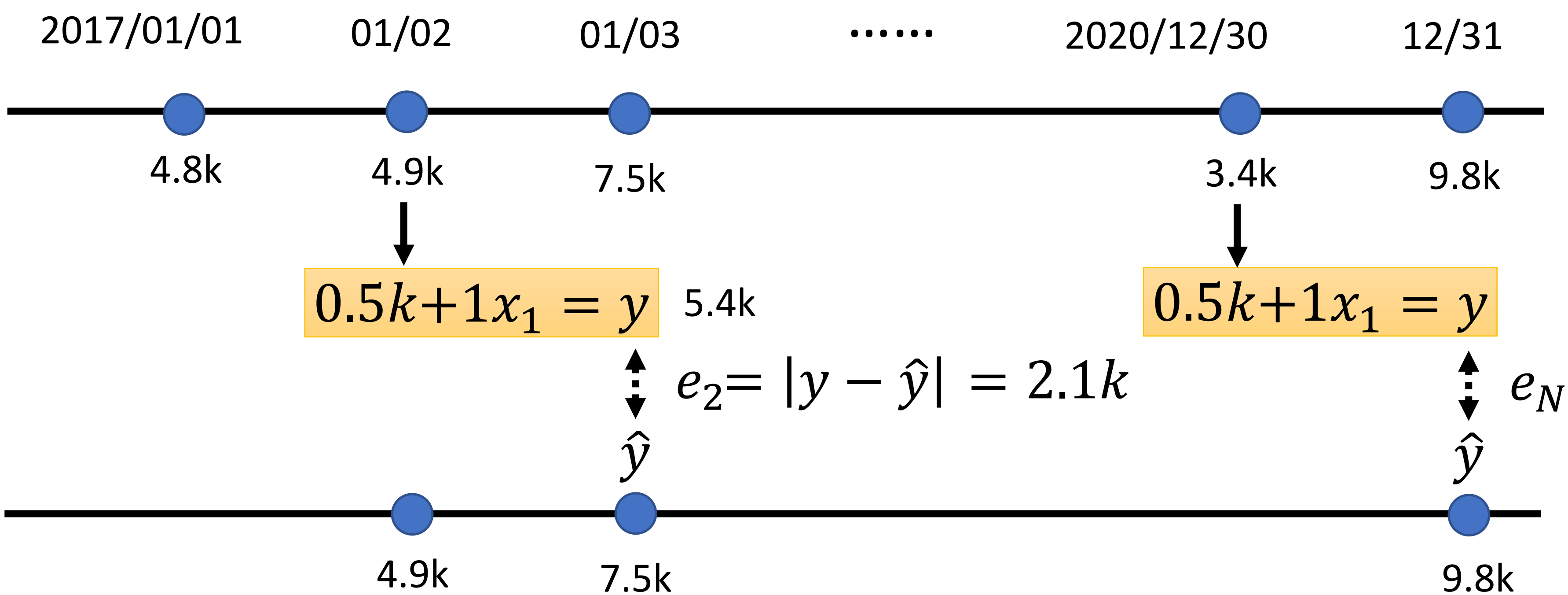

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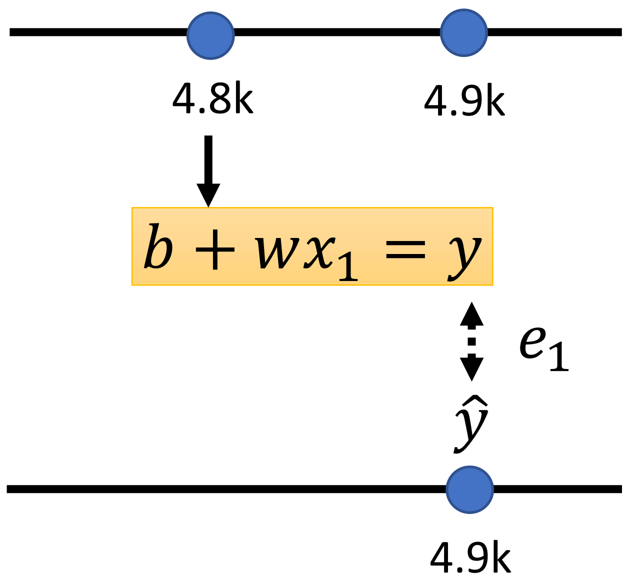


Loss: $L = \frac{1}{N}\sum_n e_n$

$e = |y - \hat{y}|$ L is mean absolute error (**MAE**)

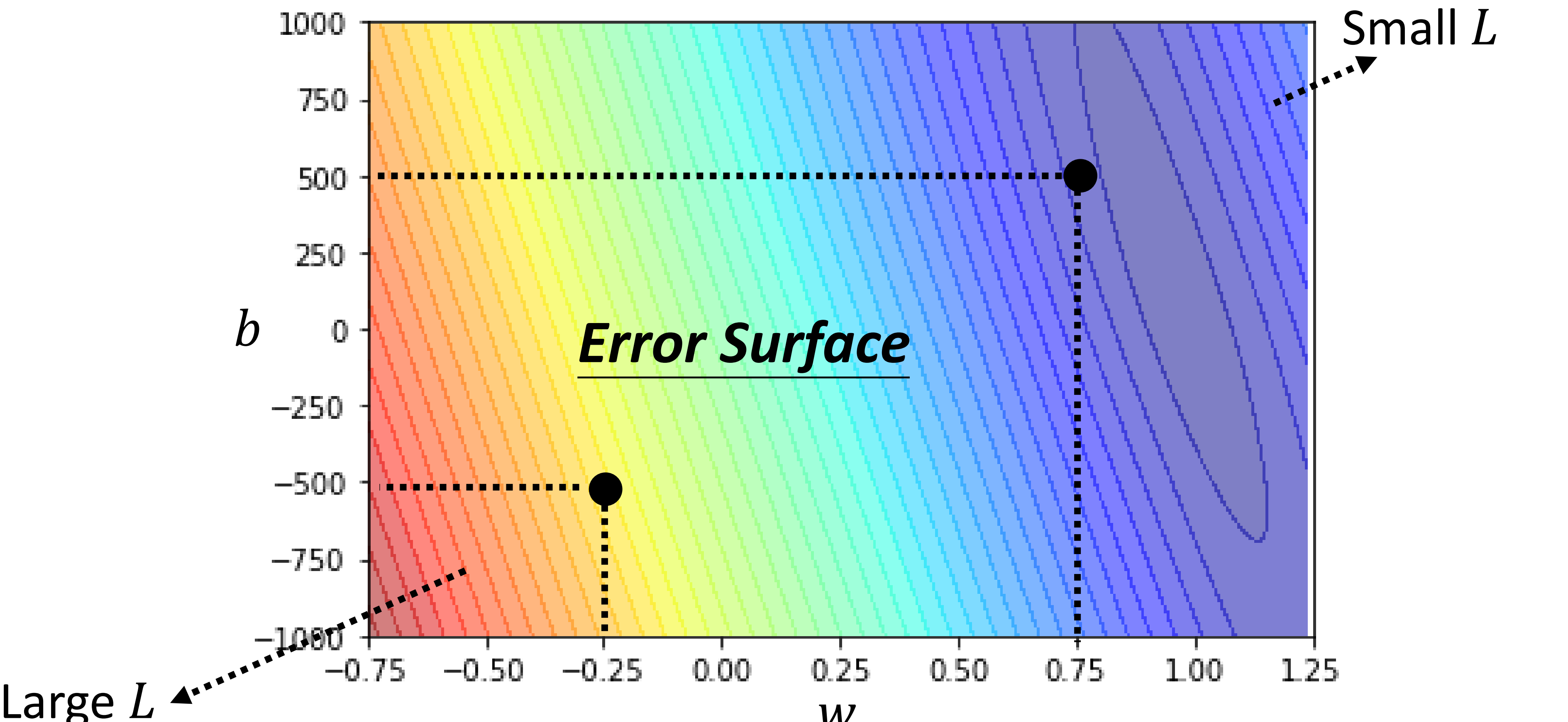
$e = (y - \hat{y})^2$ L is mean square error (**MSE**)

If y and $\hat{y}$ are both probability distributions ➡ Cross-entropy

Step2: Define Loss from Training Data

- Loss is a function of parameters $L(b, w)$
- Loss: how good a set of values is.

Model $y = b + wx_1$



Step3: Optimization

Gradient Descent
梯度下降

In 1-dimension, the derivative of a function:

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

In multiple dimensions, the gradient is the vector of (partial derivatives) along each dimension.
The slope in any direction is the dot product of the direction with the gradient.
The direction of steepest descent is the negative gradient.

Practice

Try to calculate the gradient!

$$f(x_1, x_2, x_3) = \ln(1 + \exp(-2x_1 + 3x_2 - 4x_3))$$

Today's Topics

- Regression
- Linear Regression
- ***Gradient Descent***
- Regularization

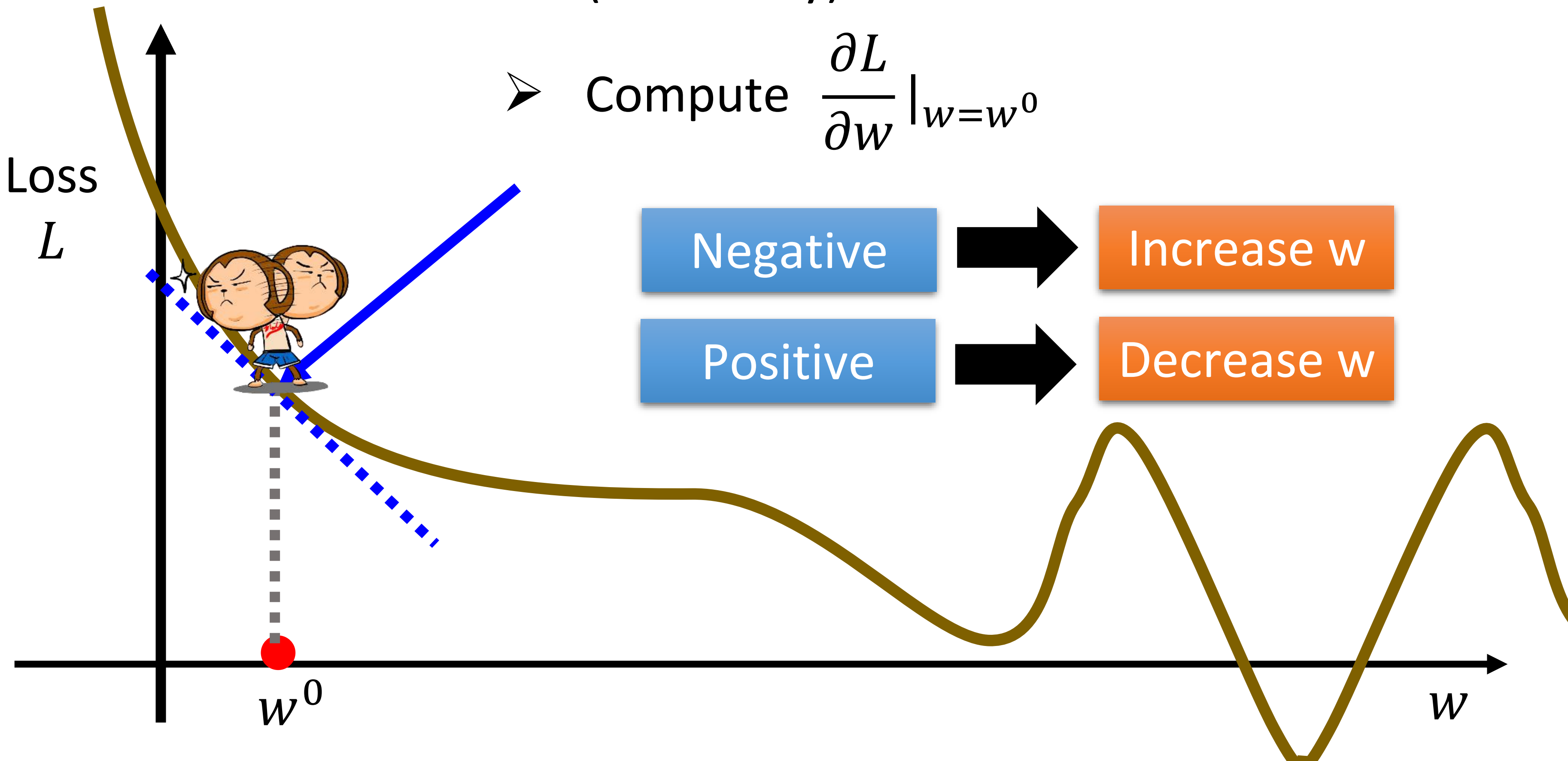
Gradient Descent

w^* [redacted] $= arg \min_{w}$ [redacted] L

- (Randomly) Pick an initial value w^0
- Compute $\frac{\partial L}{\partial w}|_{w=w^0}$

Negative → Increase w

Positive → Decrease w



Gradient Descent

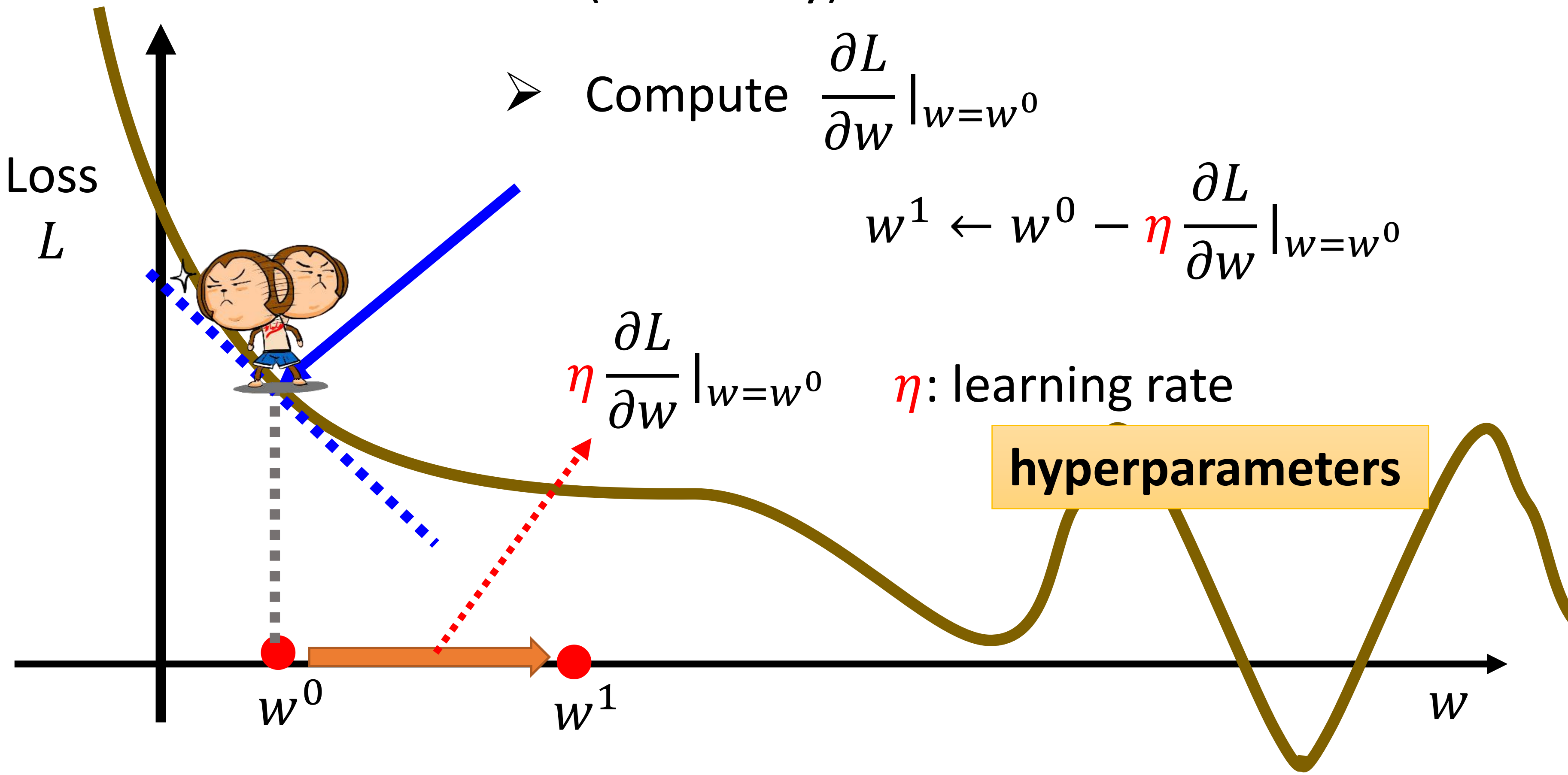
w^* [redacted] $= arg \min_{w}$ [redacted] L

- (Randomly) Pick an initial value w^0
- Compute $\frac{\partial L}{\partial w}|_{w=w^0}$

$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0}$$

η: learning rate

hyperparameters



Source of image: http://chico386.pixnet.net/album/photo/171572850

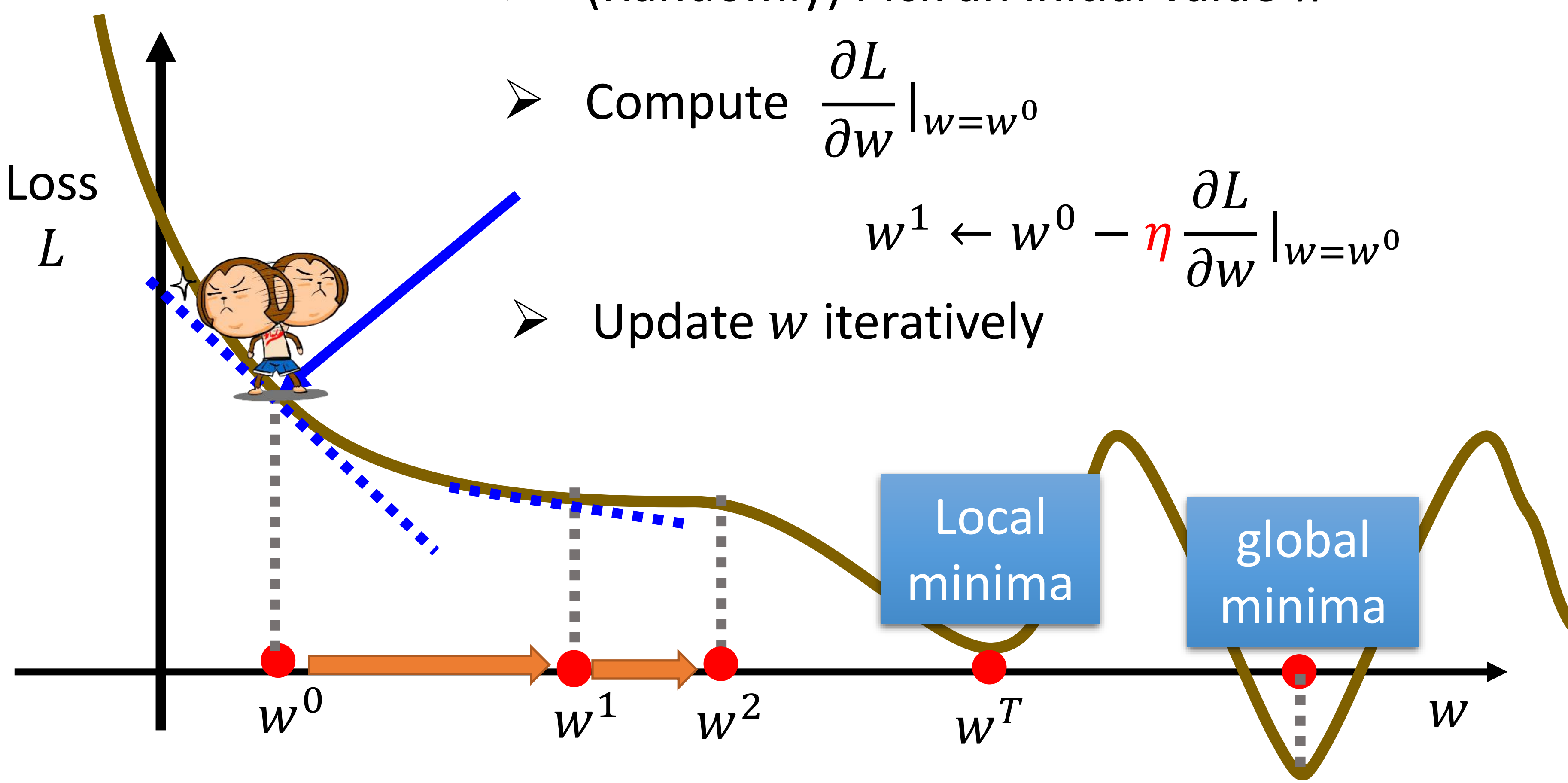
Gradient Descent

w^* [redacted] $= arg \min_{w} L$ [redacted]

- (Randomly) Pick an initial value w^0
- Compute $\frac{\partial L}{\partial w}|_{w=w^0}$

$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0}$$

- Update w iteratively



Gradient Descent

$$w^*, b^* = arg\min_{w,b} L$$

- (Randomly) Pick initial values w^0, b^0
- Compute

$$\boxed{\begin{array}{l} \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \\ \\ \frac{\partial L}{\partial b}|_{w=w^0,b=b^0} \end{array}}$$

$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0}$$

$$b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

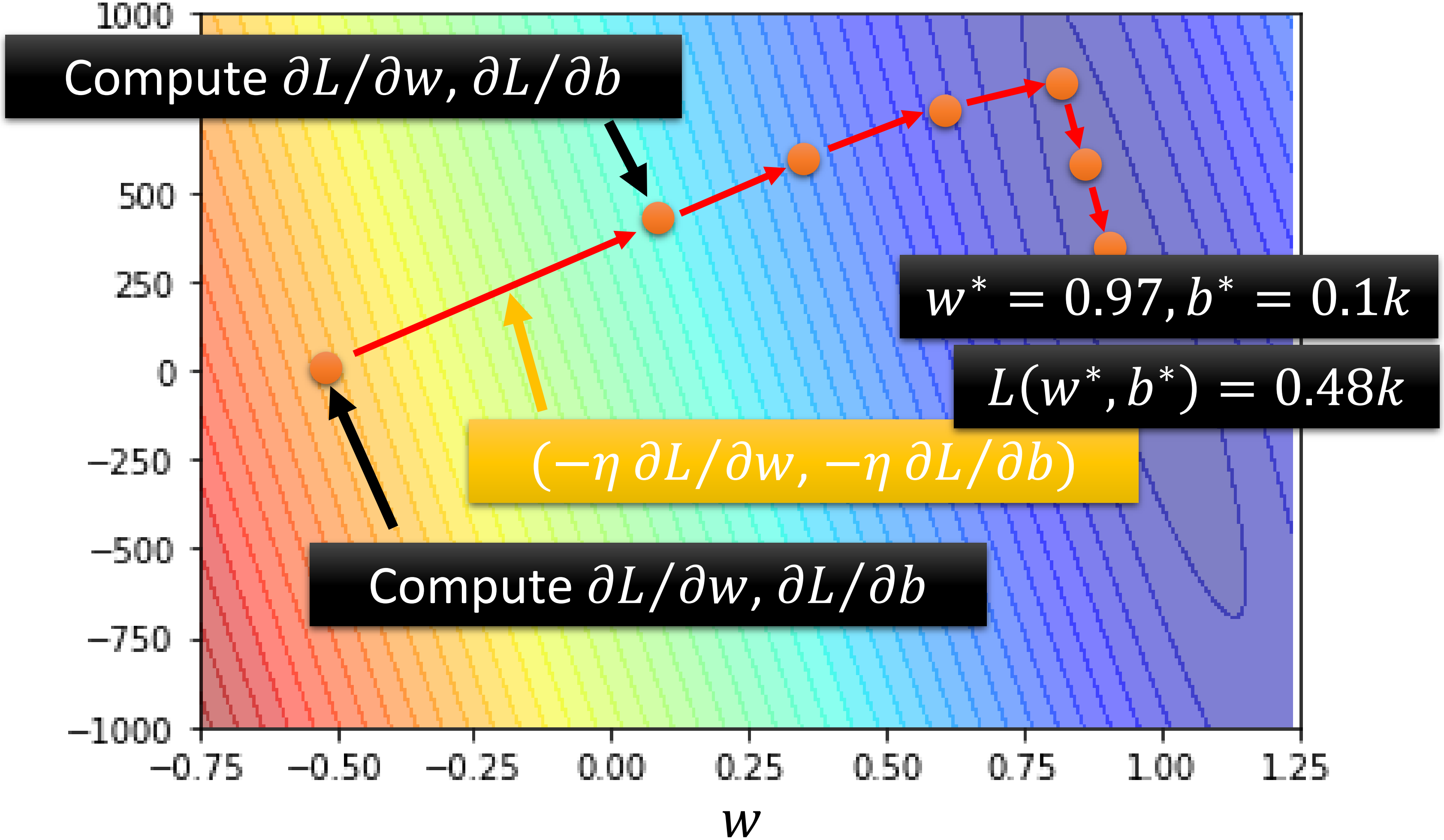
Can be done in one line in most deep learning frameworks

- Update w and b interatively

Gradient Descent

Model $y = b + wx_1$

$$w^*, b^* = arg\min_{w,b} L$$

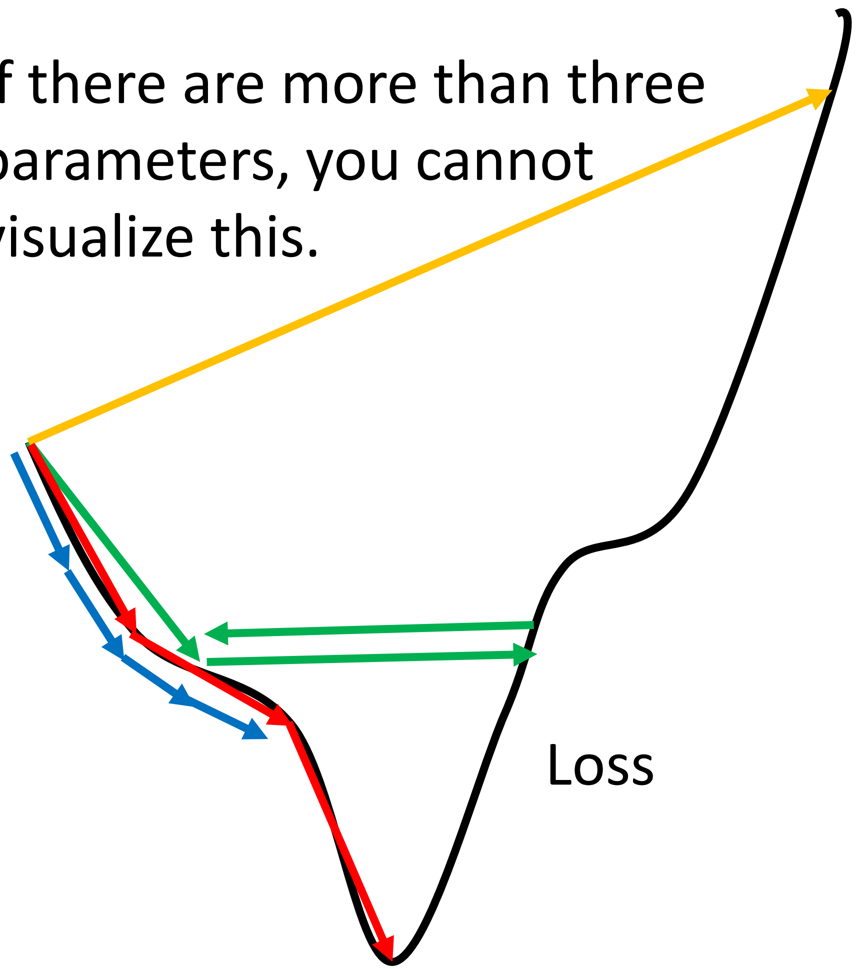


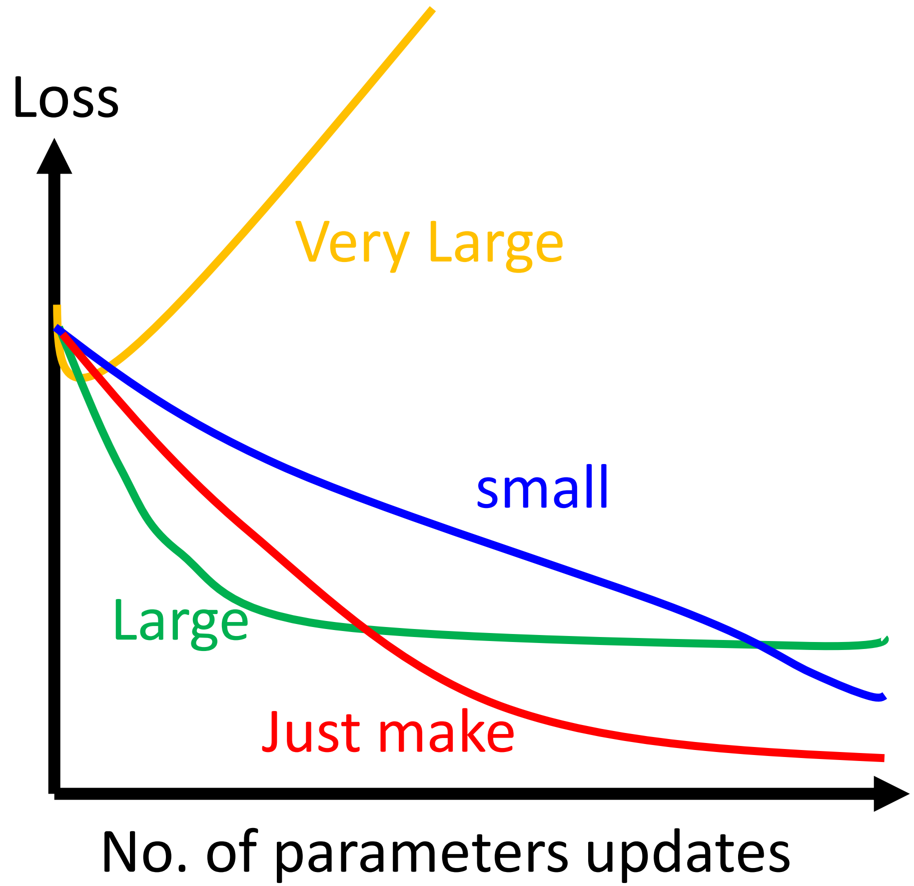
Learning Rate

$$\theta^{i} = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$$

Set the learning rate η carefully

If there are more than three parameters, you cannot visualize this.





But you can always visualize this.

Gradient Descent

Tip 1: Adaptive Learning Rate

Adaptive LR

Adagrad

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t}(g^i)^2}} g^t$$

- Popular & Simple Idea: Reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - E.g. 1/t decay: $\eta^t = \eta/\sqrt{t+1}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates

Gradient Descent

Tip 2: Stochastic Gradient Descent

Stochastic Gradient Descent (SGD)

$$L = \sum_n \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2$$

Loss is the summation over all training examples

- ***Gradient Descent*** $\theta^i = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$

- ***Stochastic Gradient Descent***

Faster!

Pick an example x^n

Loss for only one example

$$L^n = \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2 \qquad \theta^i = \theta^{i-1} - \eta \nabla L^n\left(\theta^{i-1}\right)$$

SGD

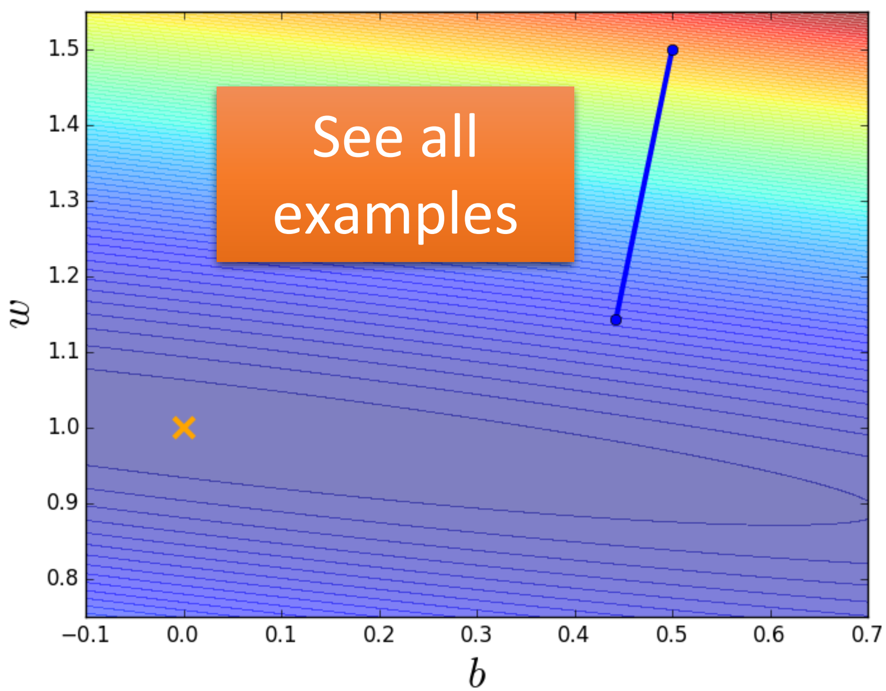
Stochastic Gradient Descent

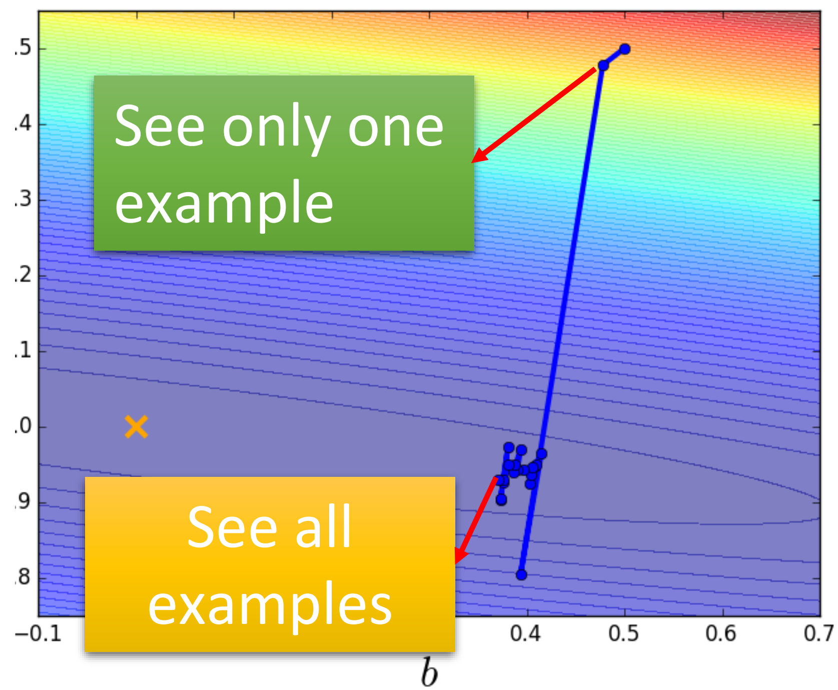
Update for each example

If there are 20 examples, 20 times faster.

Gradient Descent

Update after seeing all examples



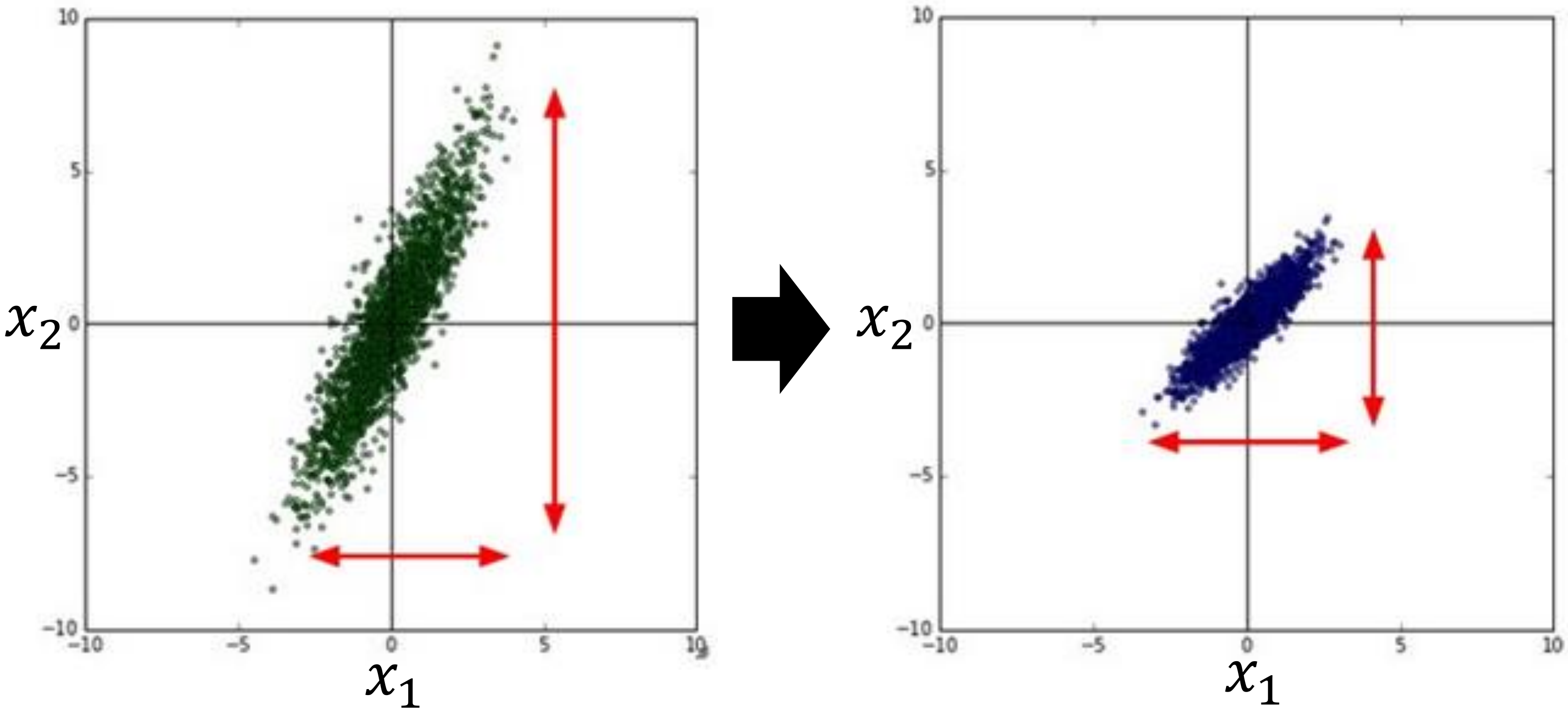


Gradient Descent

Tip 3: Feature Scaling

Feature Scaling

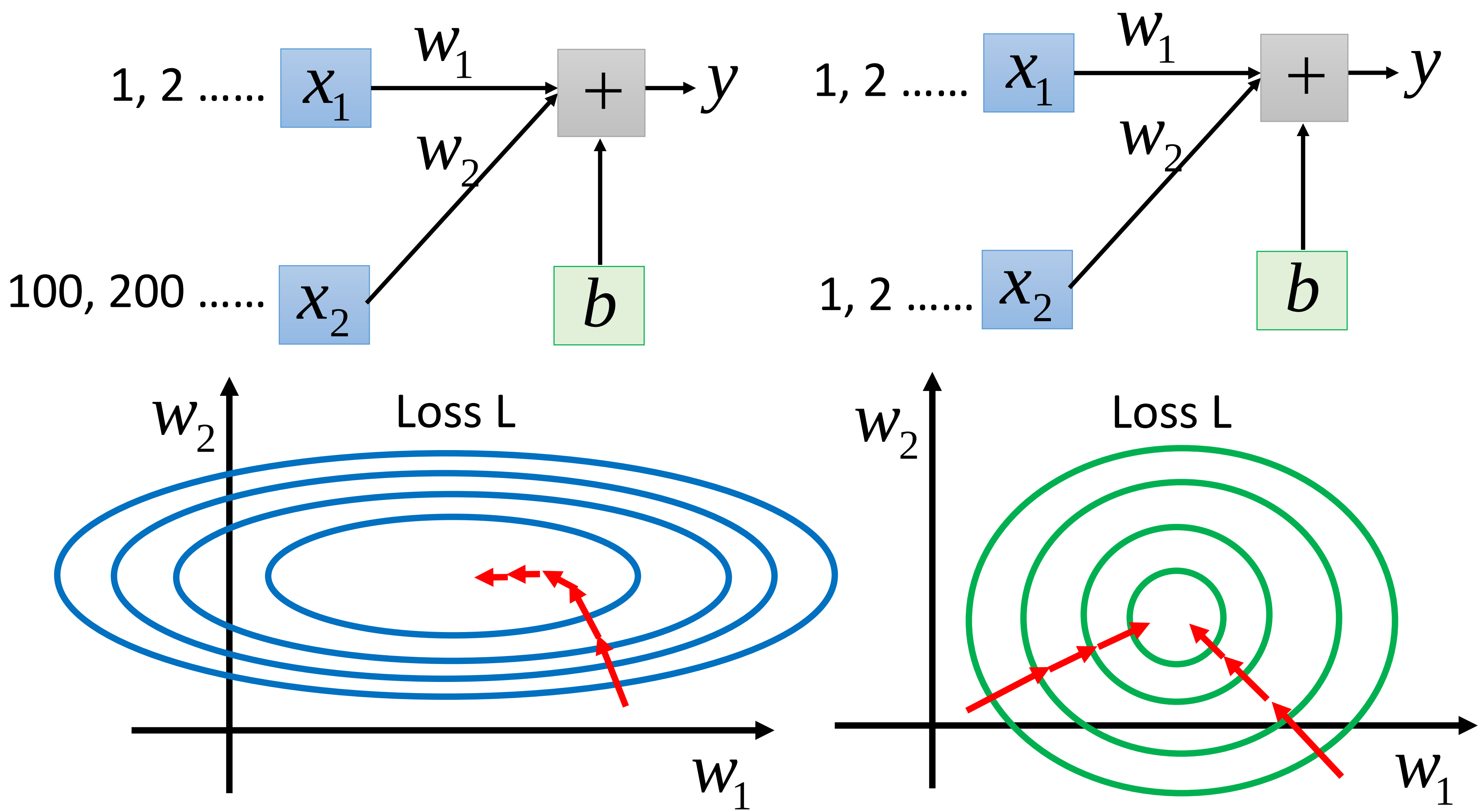
$$y = b + w_1 x_1 + w_2 x_2$$



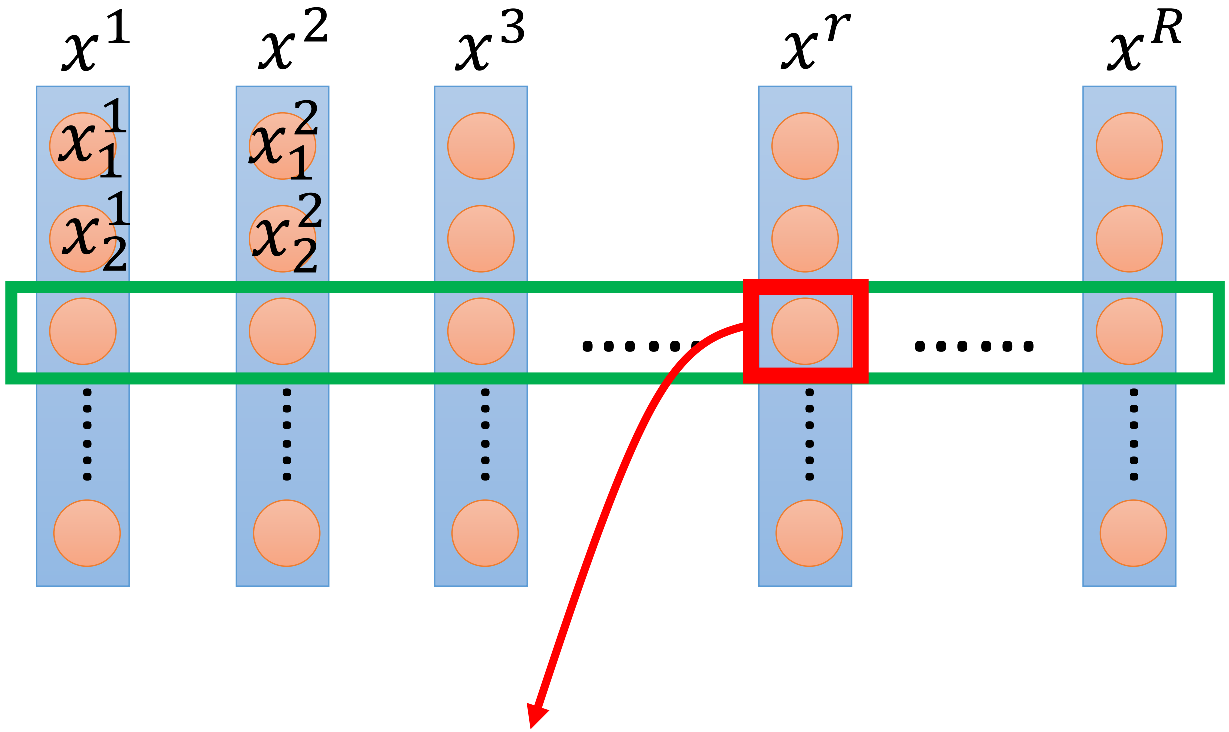
Make different features have the same scaling

Feature Scaling

$y = b + w_1 x_1 + w_2 x_2$



Feature Scaling



For each dimension i:

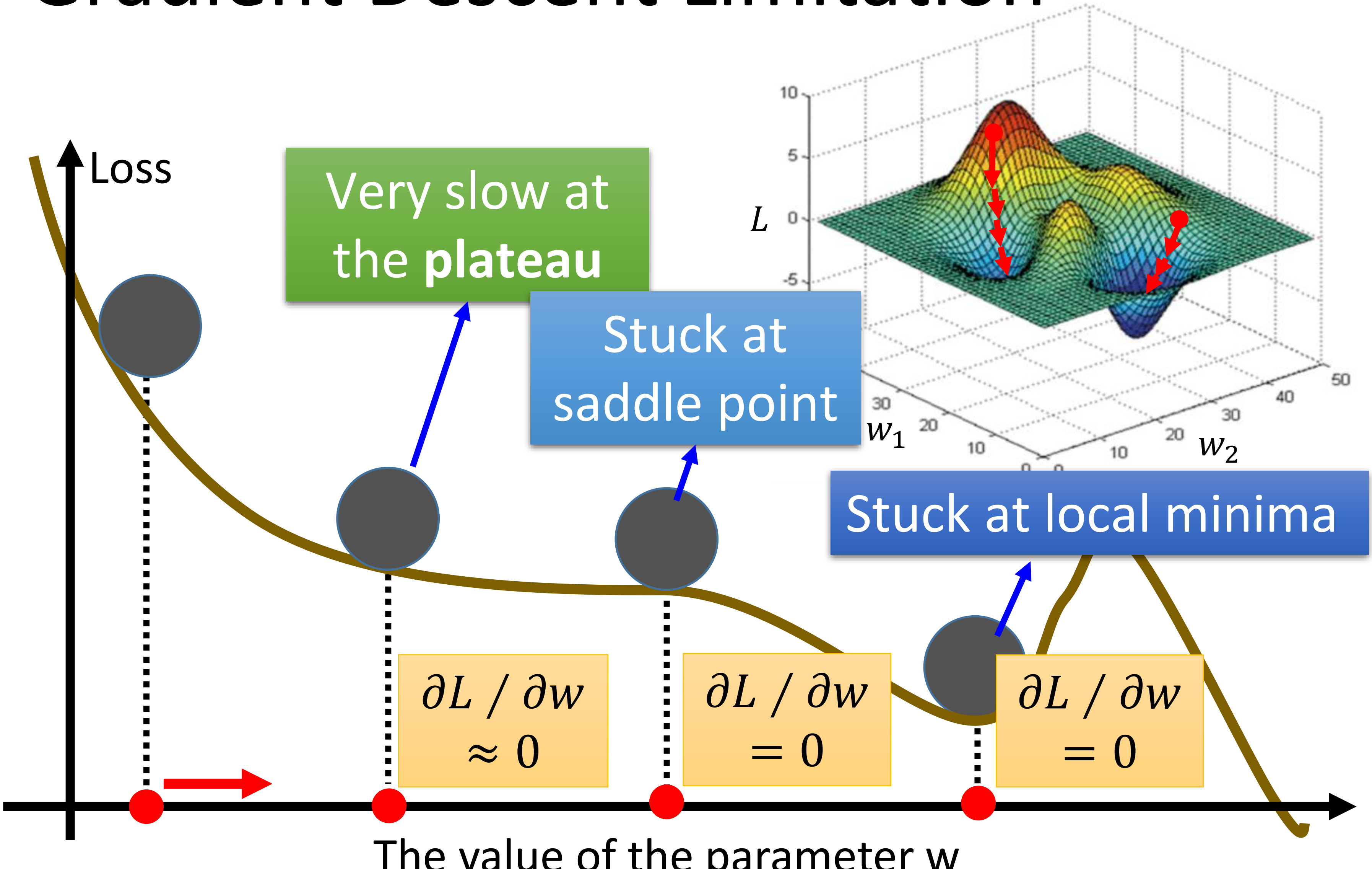
mean: m_i

standard deviation: σ_i

$$x_i^r \leftarrow \frac{x_i^r - m_i}{\sigma_i}$$

The means of all dimensions are 0, and the variances are all 1

Gradient Descent Limitation



So far, we've got optimization

Let's go back to the machine learning framework.

Machine Learning is so simple ……

$w^* = 0.97, b^* = 0.1k$

$L(w^*, b^*) = 0.48k$

$y = b + wx_1$

Step 1: function with unknown param → Step 2: define loss from training data → Step 3: optimization

Training

$y = 0.1k + 0.97x_1$ achieves the smallest loss $L = 0.48k$ on data of 2017 – 2020 (**training data**)

How about data of 2021 (**unseen during training**)?

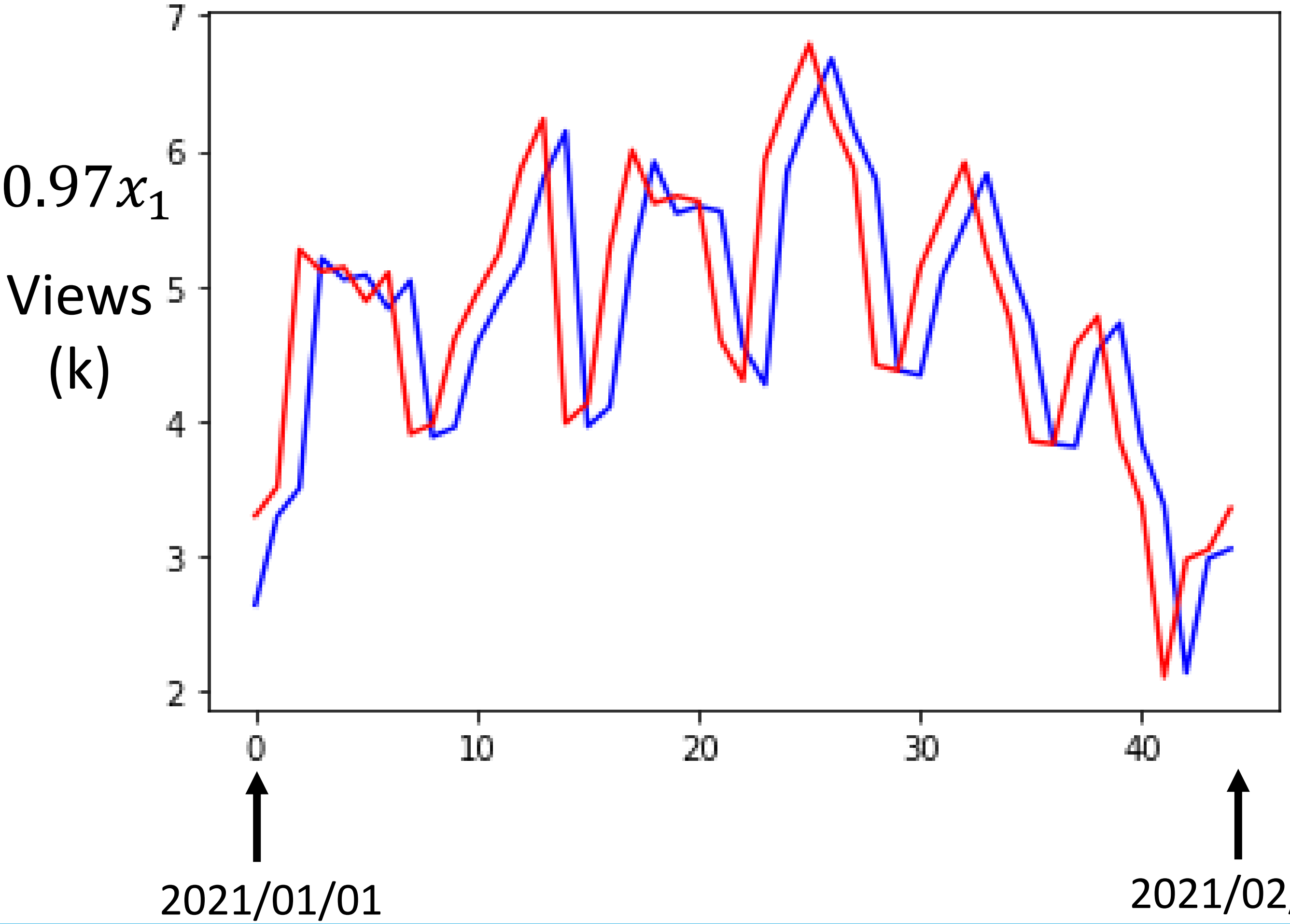
$L' = 0.58k$

The result

Red: real no. of views

blue: estimated no. of views

$$y = 0.1k + 0.97x_1$$



Linear Regression Summary

Model $y = b + wx_1$

Loss

$e = |y - \hat{y}|$ L is mean absolute error (**MAE**)

$e = (y - \hat{y})^2$ L is mean square error (**MSE**)

Optimization Gradient Descent

Linear Regression Summary

- **Strength & Weakness**

✓Easy to understand and implement

✓Good comprehensibility

✕Performs poorly when there are non-linear relationships

✕Not flexible enough to capture more complex patterns

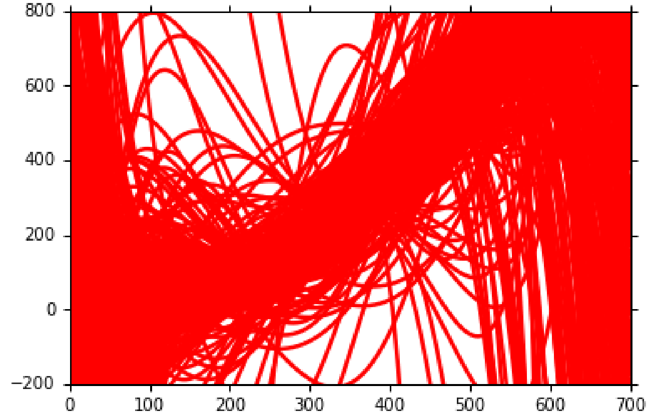
Today's Topics

- Regression
- Linear Regression
- Gradient Descent
- ***Regularization***

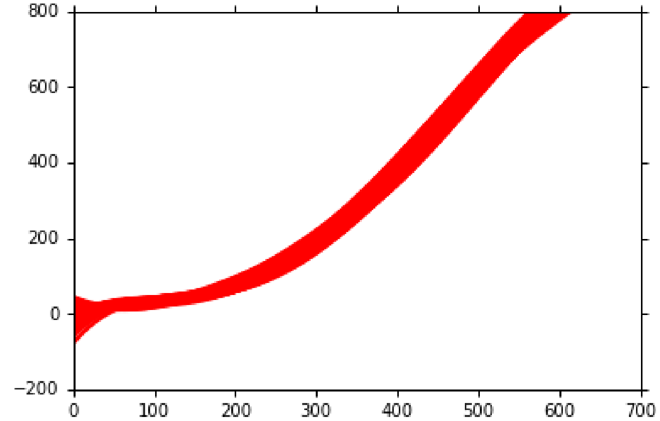
Recall: What to do with large variance?

- More data

Very effective, but not always practical

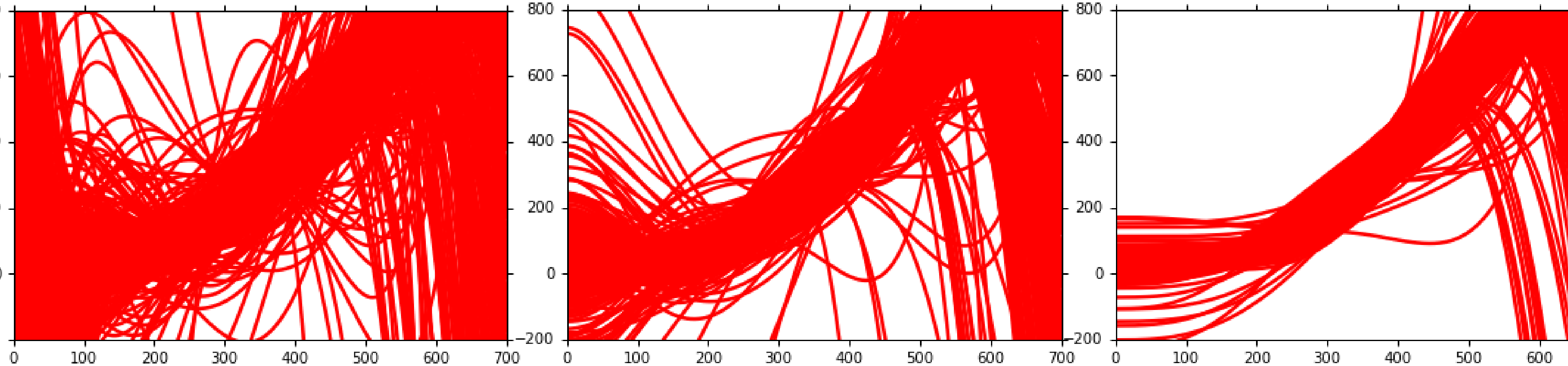


10 examples



100 examples

- ***Regularization***



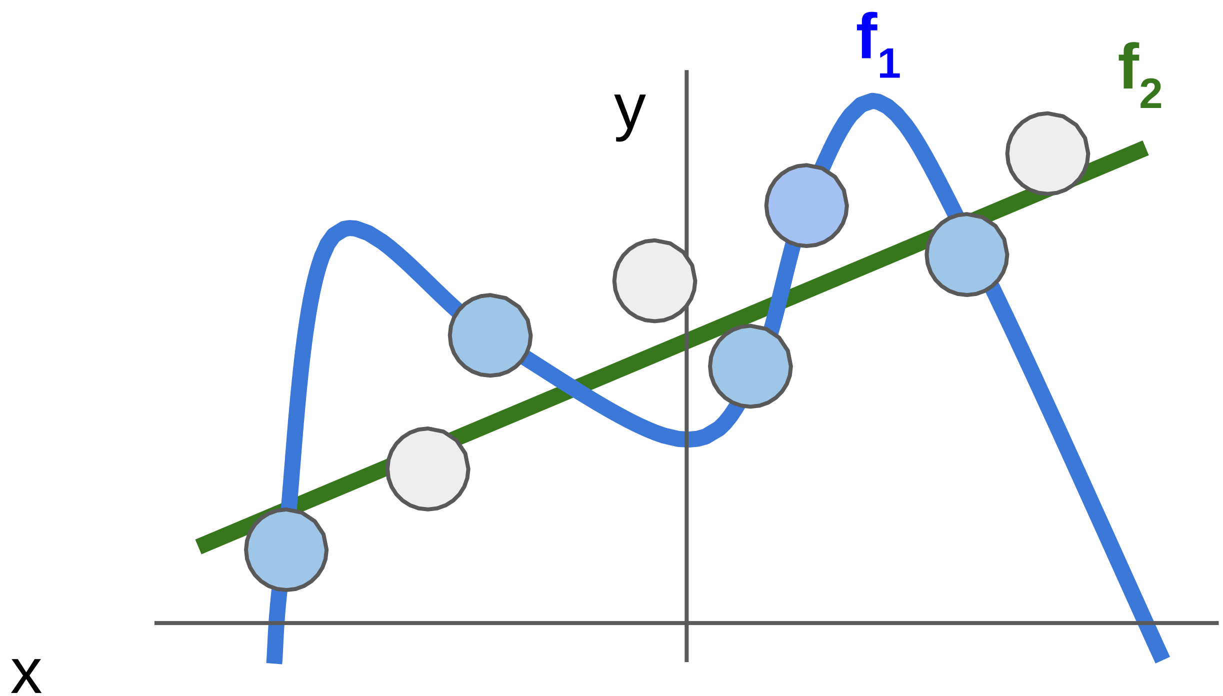
Regularization

- Complex model leads to overfitting. Regularization is a way to mitigate this undesirable behavior.
- Through regularization, we can *penalize* complex models and favor simpler ones.

$$min_w \ \mathcal{L}(w) + \Omega(w)$$

- The second term Ω is a regularizer, measuring the complexity of the model given by w.

Regularization intuition: Prefer Simpler Models



Regularization pushes against fitting the data *too* well so we don't fit noise in the data

Regularization

- **L2 Regularization**

$$\Omega(w) = \lambda \|w\|_2^2$$

$$\textit{\textbf{where}}\ \|w\|_2^2 = \Sigma_i w_i^2$$

Here the main effect is that large model weights $\boldsymbol{w_i}$ will be **penalized** (avoided), since we consider them "unlikely", while small ones are ok.

Example: ridge regression --> MSE + L2 Regularization

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \sum_{n=1}^{N} \left[y_n - \mathbf{x}_n^\top \mathbf{w} \right]^2 \ + \ \lambda \|\mathbf{w}\|_2^2$$

Regularization

- **L1 Regularization**

$$\Omega(w) = \lambda \|w\|_1$$

$$\textit{where } \|w\|_1 = \Sigma_i |w_i|$$

For the L1-regularization the optimum solution is likely going to be **sparse** (only has few non-zero components) compared to the case where we use L2-regularization.

Example: lasso regression --> MSE + L1 Regularization

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \sum_{n=1}^{N} [y_n - \mathbf{x}_n^\top \mathbf{w}]^2 \; + \; \lambda \, \|\mathbf{w}\|_1$$

Regularization

- **L0 Regularization**

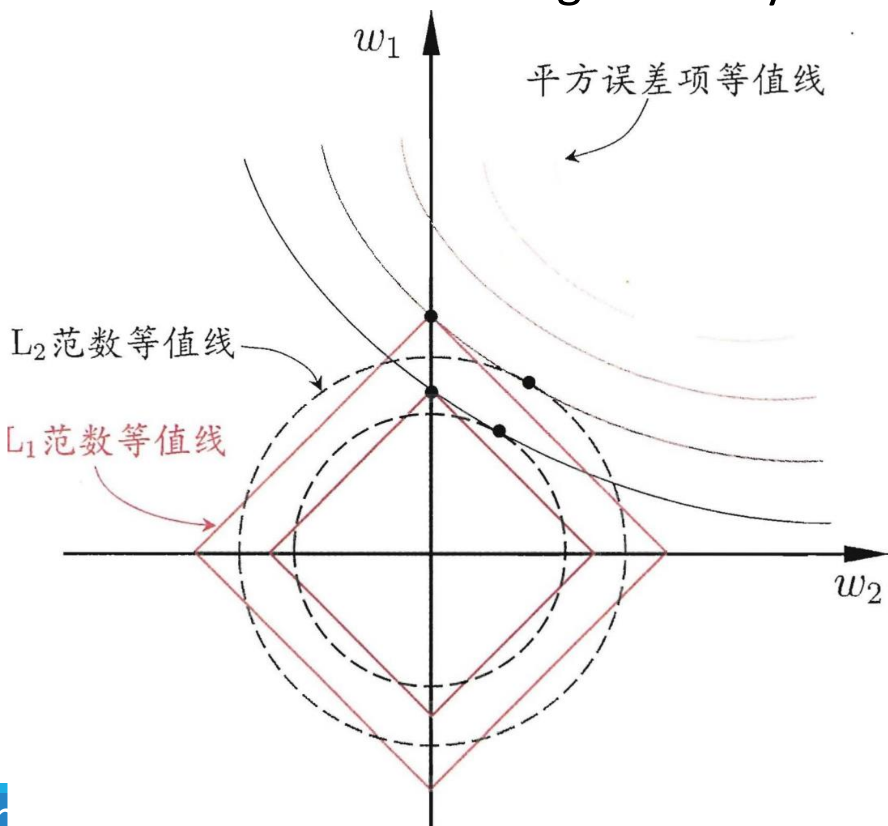
$$\Omega(w) = \lambda \|w\|_{\mathbf{0}}$$

$$\boldsymbol{where}\ \|w\|_{\mathbf{0}} = \Sigma_i |w_i|^{\mathbf{0}}$$

- Feature selection can also be achieved by using the number of non-zero parameters.
- However, L1 regularization is generally used, because the L0 norm is an NP-hard problem, and it is difficult to find the optimal solution.

L1 VS L2

- **Both** can help reduce the risk of overfitting
- **L2 Regularization** tends to distribute weights evenly among related features
- **L1 Regularization** tends to select one from the relevant features, and the rest of the feature weights decay to zero (*Feature Selection*)



L1 regularization is easier to obtain ***sparse solutions*** than L2 regularization

L1 VS L2 : Case Study

$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$

$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1^T x = w_2^T x = 1$$

Which of w1 or w2 will the L2 regularizer prefer?

L1 VS L2 : Case Study

$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$

$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1^T x = w_2^T x = 1$$

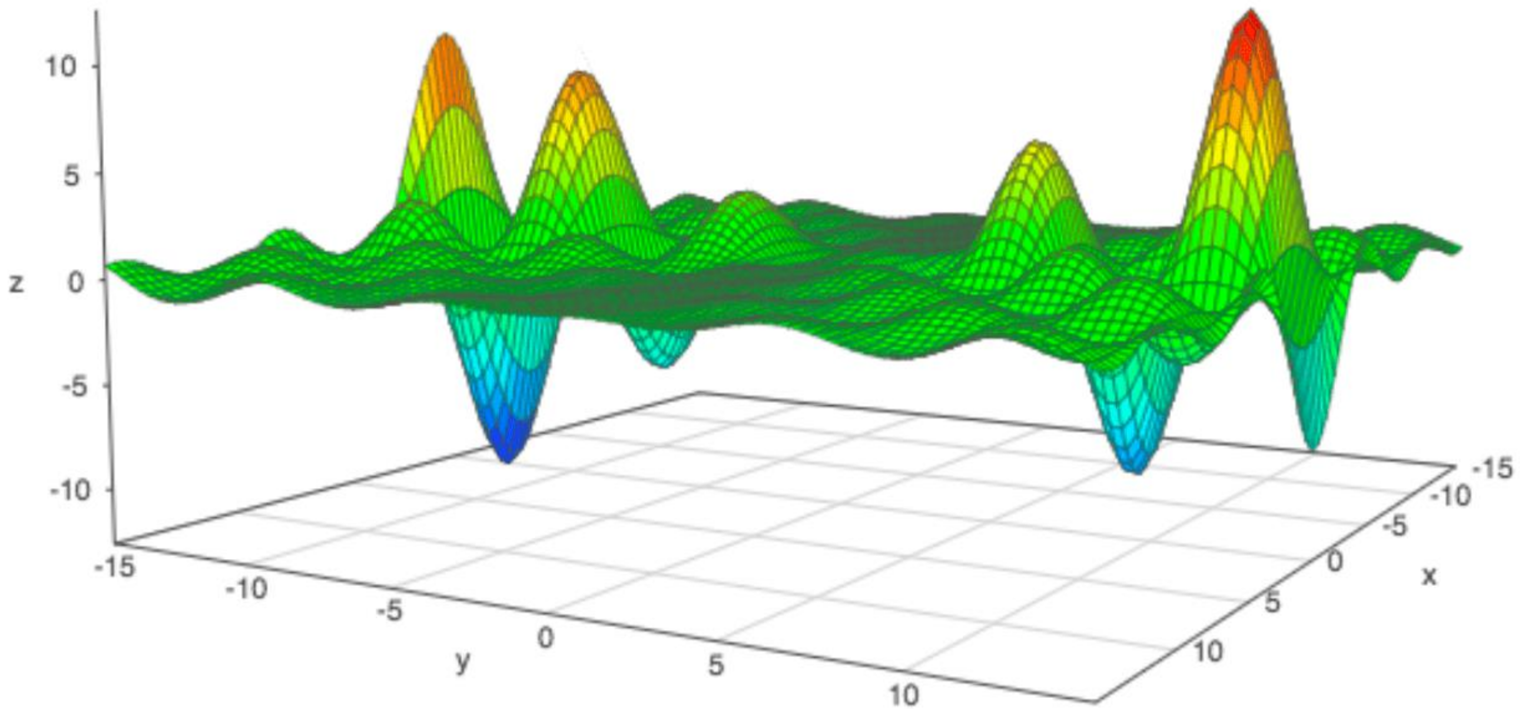
Which of w1 or w2 will the L1 regularizer prefer?

Summary

- **Regression**
  - difference with classification
- **Linear Regression**
  - model, loss and optimization
- **Gradient Descent**
  - steps, learning rate, …
- **Regularization**
  - L0 Regularization
  - L1 Regularization
  - L2 Regularization

Some questions…

- Does local minima truly cause the problem?



Some questions…

- How does learning rate η influence the optimization?