# 11-695: AI Engineering
# Supervised Learning

Spring 2019

# Outline

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# Image Classification

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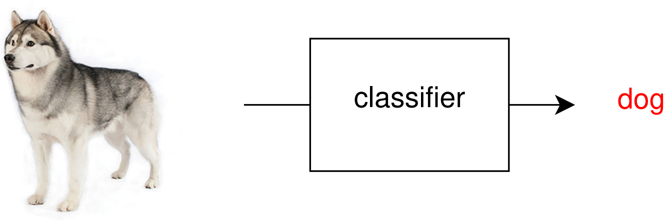
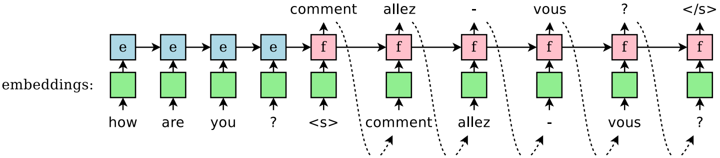
- Find a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$
  - $\mathbf{x}$: an image
  - $\mathbf{y}$: dog, cat, bird, car, etc.



# Machine Translation

- Find a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$
  - $\mathbf{x}$: an English sentence
  - $\mathbf{y}$: an French sentence



# How to Find the Function f?

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Learn from data

# Outline

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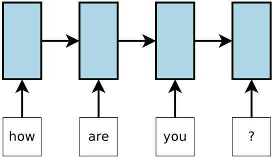
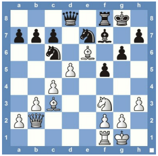
# Data and Label

- Pairs of $(\mathbf{x}, \mathbf{y})$: $\{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), ..., (\mathbf{x}^{(N)}, \mathbf{y}^{(N)})\}$
- Each $\mathbf{x}^{(i)}$ is called a *data point*
- Each $\mathbf{y}^{(i)}$ is called a *label*
- $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ can be *anything*



# Data Representation

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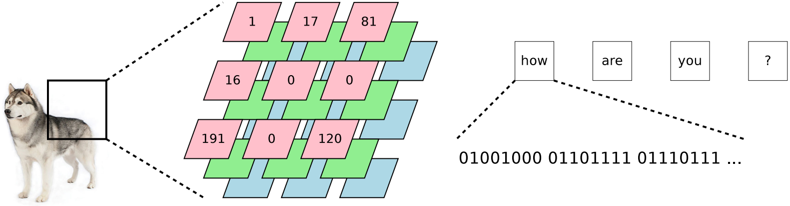

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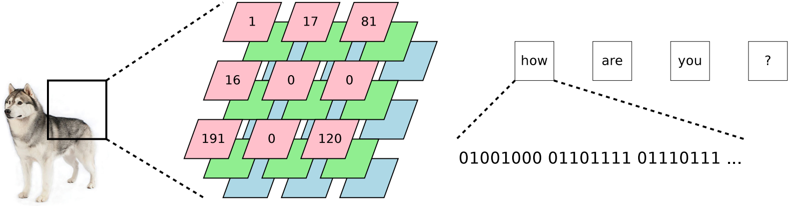


- ... so it's hard to make them think like we do

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  - *Structured prediction* problems
- Why learn these?
  - The types of problems you tackle (loosely) tell you how to design the learning models.

# Outline

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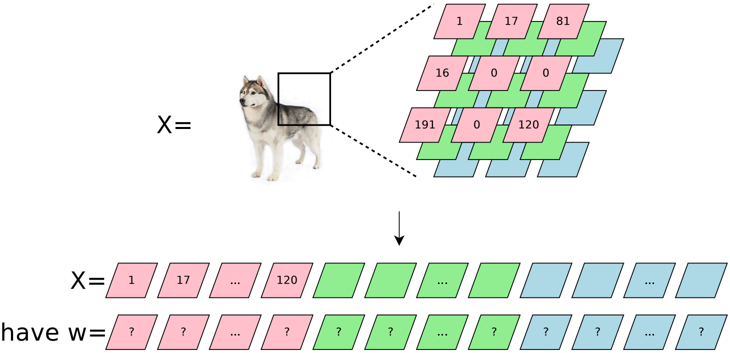
## An Example

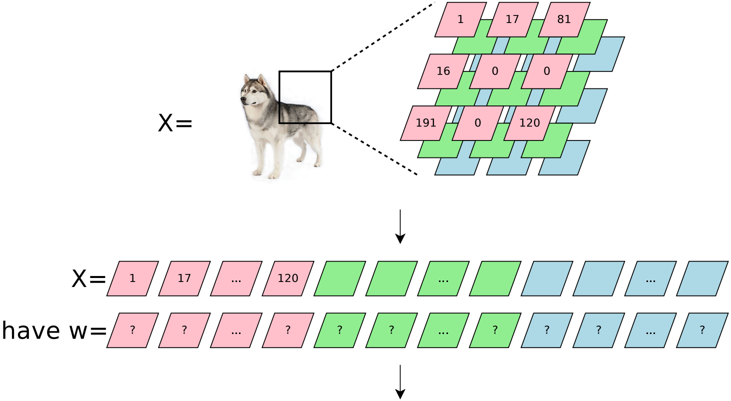
- Modeling is the process of coming up with *class of candidates*
  - Each value of $w$ gives us an $\mathbf{f}$




y = np.sum(w * x)

# An Example

- It's okay to come up with very bad classes of **f**

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  - $\mathcal{H} = \{\mathbf{f}(\mathbf{x}; \mathbf{w}) = \sum_i w_i x_i | \text{ for all } \mathbf{w}\}$
  - Each $\mathbf{w}$ gives an $\mathbf{f}$, so we write $\mathbf{y} = f(\mathbf{x}; \mathbf{w})$
  - People also write $\mathbf{y} = \mathbf{f}_{\mathbf{w}}(\mathbf{x})$ or $\mathbf{y} = \mathbf{f}^{\mathbf{w}}(\mathbf{x})$

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  - People also write $\mathbf{y} = \mathbf{f}_{\mathbf{w}}(\mathbf{x})$ or $\mathbf{y} = \mathbf{f}^{\mathbf{w}}(\mathbf{x})$
- Some times you have more than one $\mathbf{w}$. For example:
  - $\mathbf{x} \in \mathbb{R}^{1\times 100}$
  - $\mathbf{y}_1 = (\mathbf{x} \cdot \mathbf{w}_1)^2$ where $\mathbf{w}_1 \in \mathbb{R}^{100\times 200}$
  - $\mathbf{y}_2 = 1/(\mathbf{y}_1 \cdot \mathbf{w}_2)$ where $\mathbf{w}_2 \in \mathbb{R}^{100\times 1}$
  - We use $\theta$ to denote all $\mathbf{w}$'s. $\mathbf{y} = \mathbf{f}(\mathbf{x}; \mathbf{w}_1, \mathbf{w}_2) = \mathbf{f}(\mathbf{x}; \theta)$. $\theta$ is called *parameters.*

# The Bias-Variance Tradeoff

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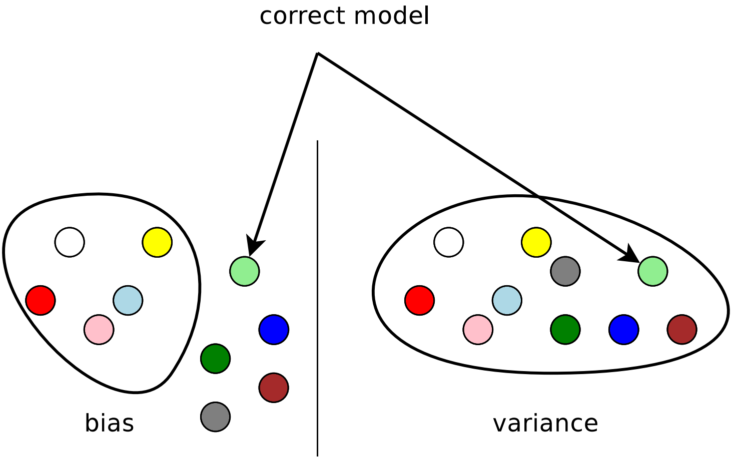
- Intuitions to design a good class of hypotheses $\mathcal{H}$
  - Bias: small $\mathcal{H}$ may leave out the correct model
  - Variance: large $\mathcal{H}$ is hard to navigate and find the correct model



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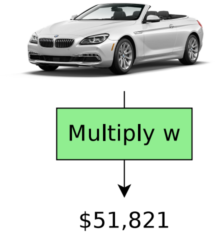

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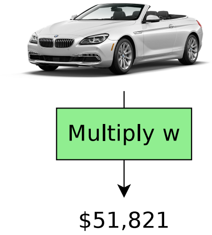

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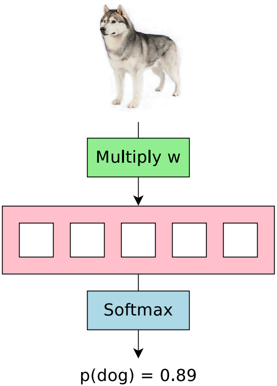

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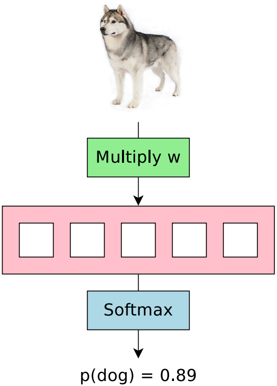
  - The function $s(\ell) = \exp\{\ell_i\} / \sum_j \exp\{\ell_j\}$ is called the *Softmax function*.



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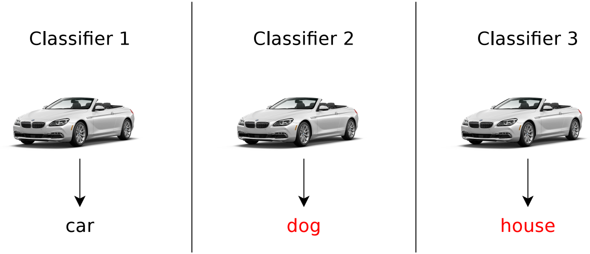
    - How about this case? Which is worse?



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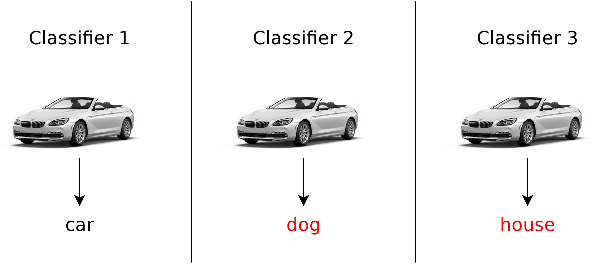


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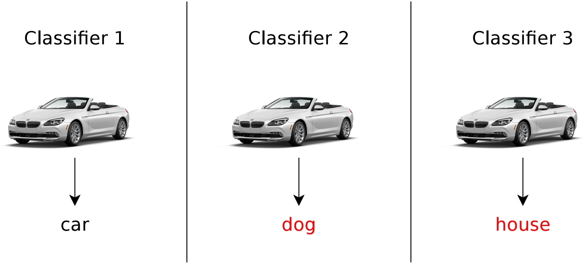


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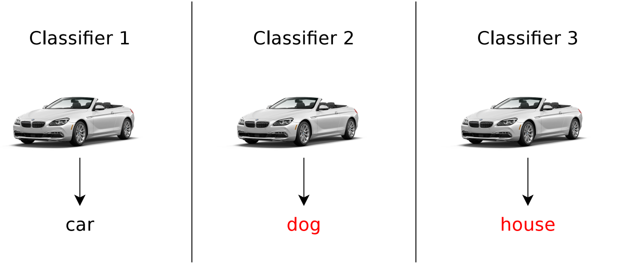


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  - How "off" is $\mathbf{y}$ from $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \theta)$

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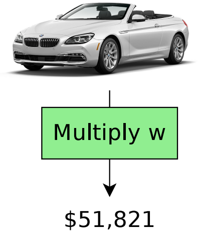

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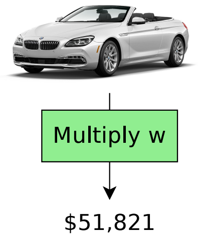

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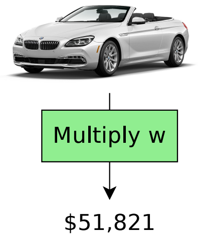
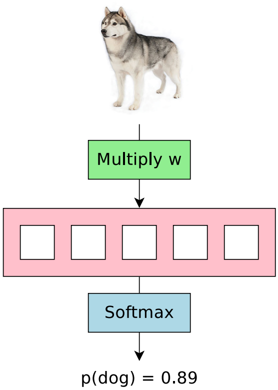
  - $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = (\hat{\mathbf{y}} - \mathbf{y})^2$ is called the $\ell_2$-*loss*
  - $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = |\hat{\mathbf{y}} - \mathbf{y}|$ is called the $\ell_1$-*loss*



# Case Study 2: Image classification

Carnegie Mellon

- Data: $\mathbf{x} \in \mathbb{R}^{3\times 32\times 32}$
- Label: $\mathbf{y} \in \{\text{dog}, \text{cat}, \text{house}, \text{car}, \text{flower}\}$
    - For ease: $\mathbf{y} \in \{1, 2, 3, 4, 5\}$
- Softmax classification:
    - Parameters: $\theta = \{\mathbf{w} \in \mathbb{R}^{3072\times 10}\}$.
    - $\mathbf{x}_1 = \text{reshape}(\mathbf{x}, [1, 3072])$
    - $\ell = \mathbf{x}_1 \cdot \mathbf{w}$
    - $\hat{p} = \mathbf{Prob}\left[\mathbf{y} = i\right] = \dfrac{\exp\{\ell_i\}}{\sum_{j=1}^{5} \exp\{\ell_j\}}$



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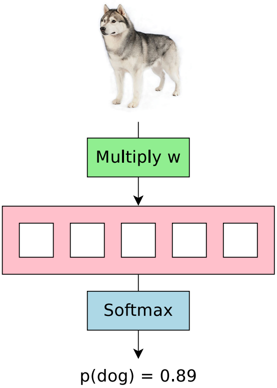

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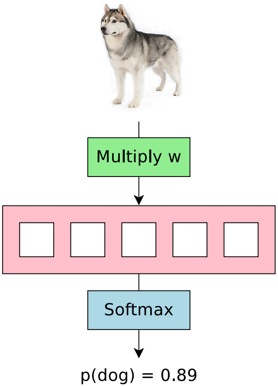

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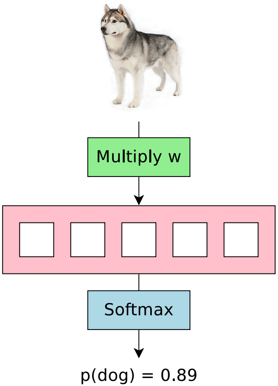

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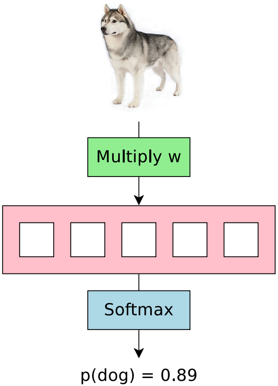

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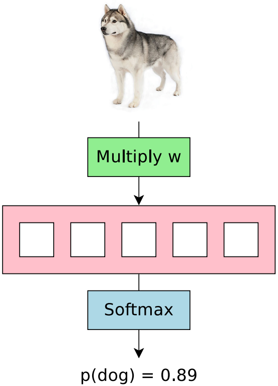

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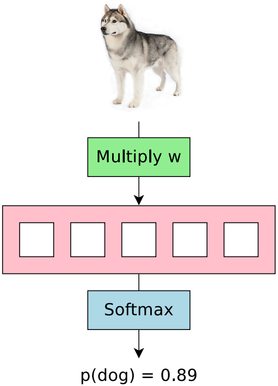

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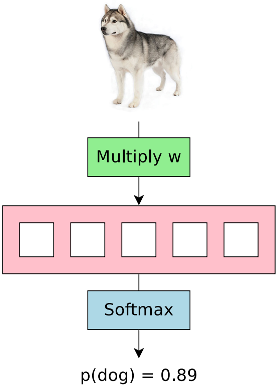
  - Making more probabilistic sense, esp. when you use sigmoid activation fuction
  - Differentiable. Recall $\hat{p}_i = \exp\{\ell_i\} / \sum_j \exp\{\ell_j\}$
    - Important for learning.



# Outline

# The Story So Far

Carnegie Mellon

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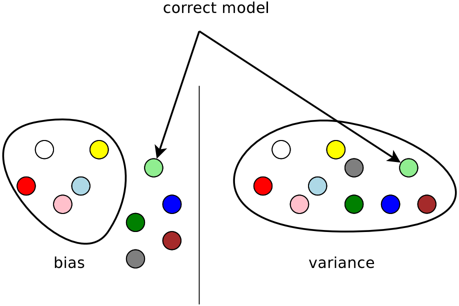

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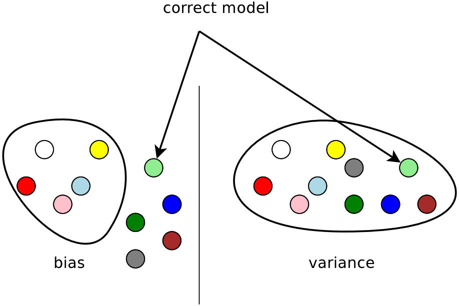
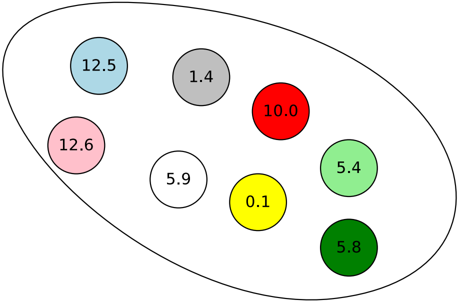



  - Come up with a *loss function* $\mathcal{L} : \mathbf{f} \in \mathcal{H} \to \mathbb{R}$, which tells you how bad is a hypothesis $\mathbf{f}$.

# Learning

- Learning is the process of finding $\mathbf{f} \in \mathcal{H}$ that minimizes $\mathcal{L}(\mathbf{f})$



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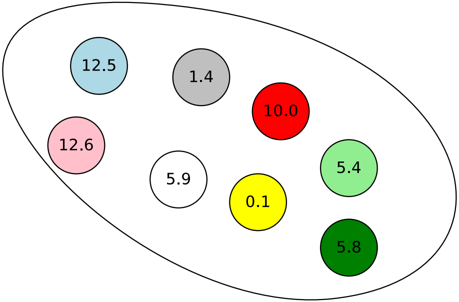


- In math: $\mathbf{f}^* = \operatorname{argmin}_{\mathbf{f} \in \mathcal{H}} \mathcal{L}(\mathbf{f})$

# Case Study: Linear Regression



- **Data:** $\{(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2), ..., (\mathbf{x}_N, \mathbf{y}_N)\}$
  - For simplicity: $\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}$.

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&= \operatorname*{argmin}_{a,b} \sum_{i=1}^{N} (a\mathbf{x}_i + b - \mathbf{y}_i)^2
\end{aligned}
$$

# Case Study: Linear Regression



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Carnegie Mellon

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- **Approach:** Find *gradients* and set to 0

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\frac{\partial \ell}{\partial b} &= \sum_{i=1}^{N} (a\mathbf{x}_i + b - \mathbf{y}_i)
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- This is a linear system in $a$, $b$. You can solve it!

# Case Study: Linear Regression



- **Approach:** Find *gradients* and set to 0

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$$\frac{\partial \ell}{\partial b} = \sum_{i=1}^{N} (a\mathbf{x}_i + b - \mathbf{y}_i)$$

$$= a\sum_{i=1}^{N} \mathbf{x}_i + b \cdot N - \sum_{i=1}^{N} \mathbf{y}_i$$

- This is a linear system in $a$, $b$. You can solve it!

# Learning is not Always Easy!



- Sometimes setting gradients to 0 does not work
  - The system does not have any solution
  - Too complicated to solve
- Neural networks: millions of parameters
  - or more extreme... (Shazeer et al., 2017)

| | Test Perplexity 10 epochs | Test Perplexity 100 epochs | #Parameters excluding embedding and softmax layers |
|---|---|---|---|
| Best Published Results | 34.7 | 30.6 | 151 million |
| Low-Budget MoE Model | 34.1 | | 4303 million |
| Medium-Budget MoE Model | 31.3 | | 4313 million |
| High-Budget MoE Model | **28.0** | | 4371 million |

- You simply *cannot* find $\mathbf{f}^* = \operatorname{argmin}_{\mathbf{f} \in \mathcal{H}} \mathcal{L}(\mathbf{f})$
- Rely on *numerical optimization algorithms.*

# Gradient Descent

Carnegie Mellon

- Data: $\left\{\left(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}\right), \left(\mathbf{x}^{(2)}, \mathbf{y}^{(2)}\right), ..., \left(\mathbf{x}^{(N)}, \mathbf{y}^{(N)}\right)\right\}$
- Hypotheses: $\mathcal{H} = \{\mathbf{f}(\mathbf{x}; \theta) : \theta \in \mathbb{R}^D\}$
- Loss function

$$\ell(\theta) = \sum_{i=1}^{N} \mathcal{L}(\mathbf{f}(\mathbf{x}_i; \theta), \mathbf{y}_i)$$

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- Gradient Descent (GD) algorithm
    - Randomly *initialize* $\theta_0 \in \mathbb{R}^D$.
    - Repeat until convergence
        - Compute the gradient: $\nabla_\theta \ell(\theta^{(t)})$
        - Update: $\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \nabla_\theta \ell(\theta^{(t)})$

# Problems with Gradient Descent

Carnegie Mellon

- We have to compute

$$\nabla_\theta \ell(\theta^{(t)}) = \nabla_\theta \sum_{i=1}^{N} \mathcal{L}(\mathbf{f}(\mathbf{x}_i; \theta), \mathbf{y}_i)$$

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- It's *very slow* if $N$ is large.
  - ImageNet: $N = 1,200,000$
  - English-German translation: $N = 4,500,000$
  - Google 1-billion-words data: $N = 1,000,000,000$
  - Human Genes: $N =$???

# Solution: Stochastic Gradient Descent



- Data: $\left\{\left(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}\right), \left(\mathbf{x}^{(2)}, \mathbf{y}^{(2)}\right), ..., \left(\mathbf{x}^{(N)}, \mathbf{y}^{(N)}\right)\right\}$
- Hypotheses: $\mathcal{H} = \{\mathbf{f}(\mathbf{x};\theta) : \theta \in \mathbb{R}^D\}$
- Loss function

$$\ell(\theta) = \sum_{i=1}^{N} \mathcal{L}(\mathbf{f}(\mathbf{x}_i;\theta), \mathbf{y}_i)$$

- Stochastic Gradient Descent (SGD) algorithm
  - Randomly *initialize* $\theta_0 \in \mathbb{R}^D$.
  - Repeat until convergence
    - Sample $(\mathbf{x}_1, \mathbf{y}_1), ..., (\mathbf{x}_B, \mathbf{y}_B)$ from your data
    - Compute the stochastic gradient:

$$\hat{\nabla}_\theta = \sum_{i=1}^{B} \nabla_\theta \mathcal{L}(\mathbf{f}(\mathbf{x}_i;\theta), \mathbf{y}_i)$$

    - Update: $\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \hat{\nabla}_\theta$

# Notes on Stochastic Gradient Descent



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    - Update: $\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \hat{\nabla}_\theta$
- You **have to** *really* sample $(\mathbf{x}_1, \mathbf{y}_1), ..., (\mathbf{x}_B, \mathbf{y}_B)$ from your data
  - otherwise, your gradient is *biased.*
  - References: Lyapunov functions; Leon Bottou's PhD thesis.

# Variations of SGD



- SGD so far:
  - Randomly *initialize* $\theta_0 \in \mathbb{R}^D$.
  - Repeat until convergence
    - Sample $(\mathbf{x}_1, \mathbf{y}_1), ..., (\mathbf{x}_B, \mathbf{y}_B)$ from your data
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- In TensorFlow: `tf.train.GradientDescentOptimizer`
- Assuming that you have a gradient $\nabla_\theta$

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    - Sample $(\mathbf{x}_1, \mathbf{y}_1), ..., (\mathbf{x}_B, \mathbf{y}_B)$ from your data
    - Compute the stochastic gradient:

$$\hat{\nabla}_\theta = \sum_{i=1}^{B} \nabla_\theta \mathcal{L}(\mathbf{f}(\mathbf{x}_i; \theta), \mathbf{y}_i)$$

    - Update: $\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \hat{\nabla}_\theta$
- In TensorFlow: `tf.train.GradientDescentOptimizer`
- Assuming that you have a gradient $\nabla_\theta$
- There are many other ways to update, more than just

$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \nabla_\theta$$

# Momentum

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- Keeps a *running average* of $\nabla_\theta$

$$v^{(t+1)} \leftarrow (1-m)v^{(t)} + m \cdot \nabla_\theta$$
$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta v^{(t+1)}$$

- You have to choose $m, \eta$
- In TensorFlow: `tf.train.MomentumOptimizer`

# Adaptive Stochastic Gradient Descent (AdaGrad)



- Keeps a *running average* of $\nabla_\theta^2$

$$v^{(t+1)} \leftarrow (1-m)v^{(t)} + m \cdot \nabla_\theta^2$$
$$\theta^{(t+1)} \leftarrow \theta^{(t)} - \eta \cdot \frac{\nabla_\theta}{\sqrt{v^{(t+1)}}}$$

- You have to choose $m, \eta$
- In TensorFlow: `tf.train.AdagradOptimizer`

# Outline

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# Is it good to minimize loss function?

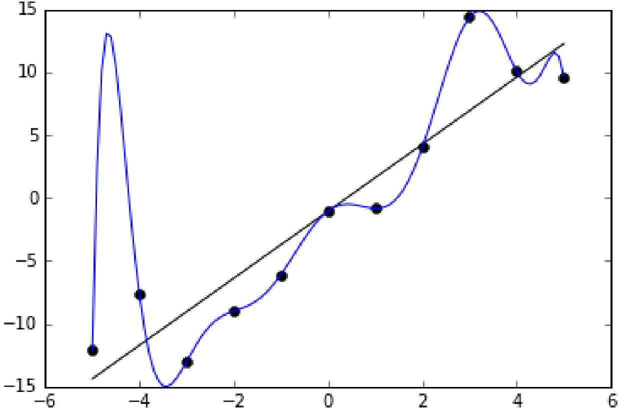


Image credit: wikipedia

# Is it good to minimize loss function?

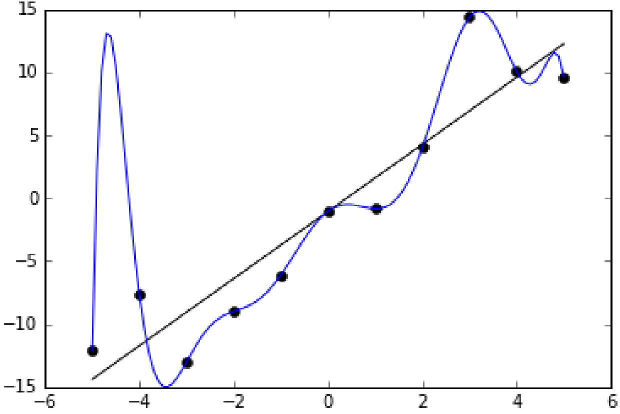


Image credit: wikipedia

- NO!

# Regularization

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- Suppose your loss function is $\ell(\theta)$
- Change it into

$$\ell^{\text{reg}}(\theta) = \ell(\theta) + \beta \|\theta\|$$

- You have to choose $\beta$
- The term $\beta \|\theta\|^2$ is called the $\ell$-2 regularization.

# Regularization

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- There are other choices
- $\ell$-1 regularization

$$\ell^{\text{reg}}(\theta) = \ell(\theta) + \beta|\theta|^2$$

- $\ell$-$p$ regularization

$$\ell^{\text{reg}}(\theta) = \ell(\theta) + \beta\left(\sum_{i=1}^{D} \theta_i^p\right)^{1/p}$$

- DropOut, DropConnect, Variational Regularization

$$\ell^{\text{reg}}(\theta) = \ell(g(\theta)),$$

where $g(\theta)$ "corrupts" $\theta$.