11-695: Competitive Engineering
Supervised Learning

Spring 2018

Outline

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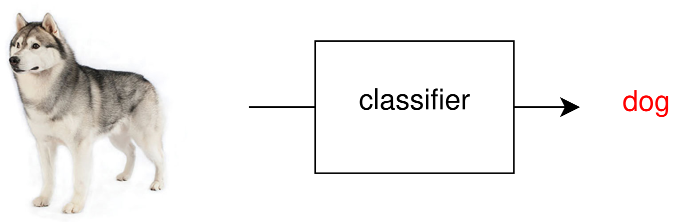
1. The Learning Problem
2. Data and Label
3. Modeling
4. Error and Loss Function
5. Learning
6. Overfitting and Regularization

Image Classification

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



Machine Translation

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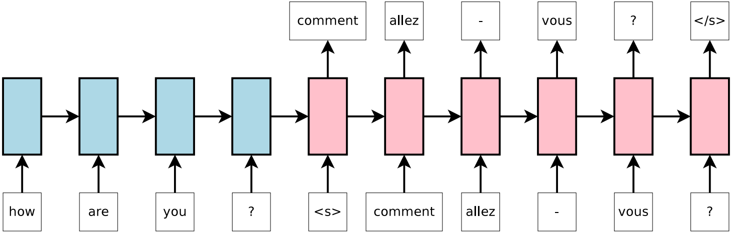
- Find a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$
  - $\mathbf{x}$: an English sentence
  - $\mathbf{y}$: an French sentence



How to Find the Function f?

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Learn from data

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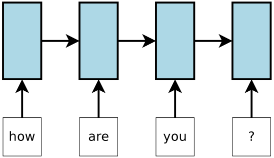
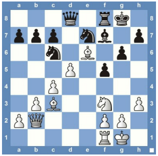
Data and Label

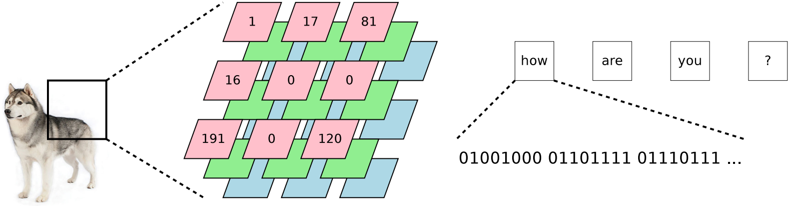
- Pairs of $(\mathbf{x}, \mathbf{y})$: $\{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), ..., (\mathbf{x}^{(N)}, \mathbf{y}^{(N)})\}$
- Each $\mathbf{x}^{(i)}$ is called a *data point*
- Each $\mathbf{y}^{(i)}$ is called a *label*
- $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$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





Data Representation

- Computers don't "see" things like we do



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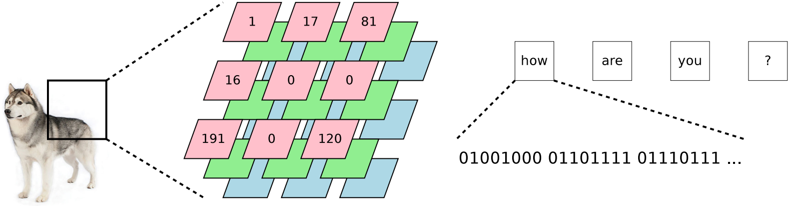

- ... so it's hard to make them think like we do

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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.

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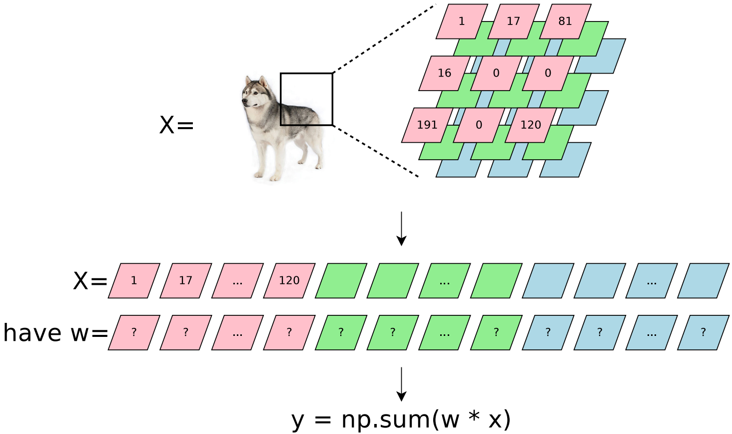
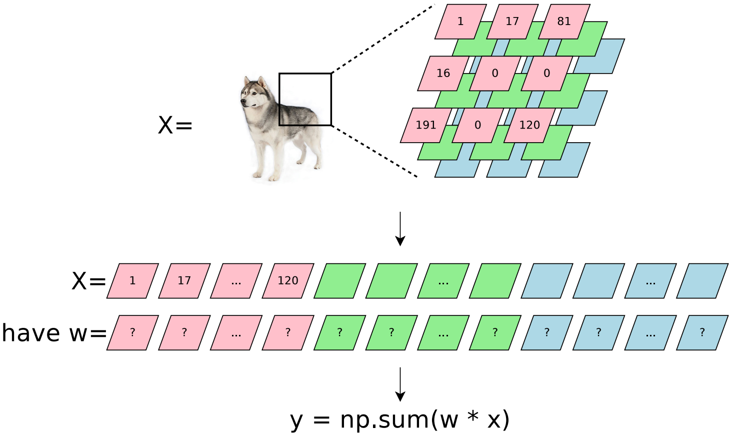
An Example

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



An Example

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



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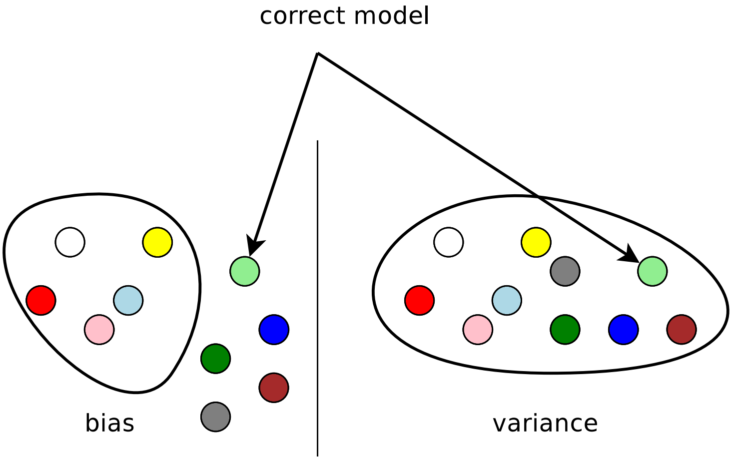
  - People also write $\mathbf{y} = \mathbf{f}_{\mathbf{w}}(\mathbf{x})$ or $\mathbf{y} = \mathbf{f}^{\mathbf{w}}(\mathbf{x})$
- Some times you have more than one $\mathbf{w}$. For example:
  - $\mathbf{x} \in \mathbb{R}^{1\times 100}$
  - $\mathbf{y}_1 = (\mathbf{x} \cdot \mathbf{w}_1)^2$ where $\mathbf{w}_1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

The Bias-Variance Tradeoff

- 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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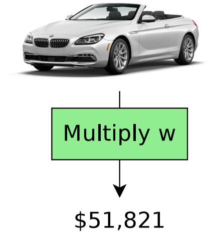

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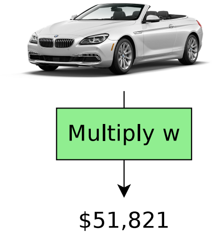

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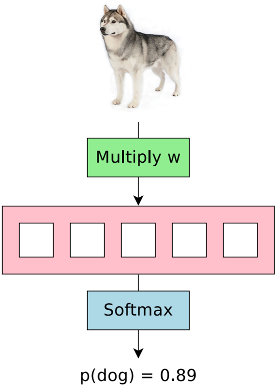

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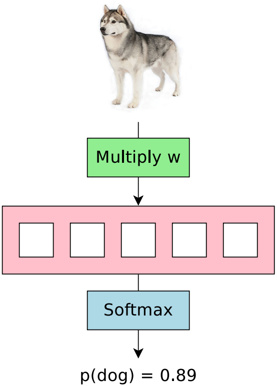
    - The function $s(\ell) = \exp\{\ell_i\} / \sum_j \exp\{\ell_j\}$ is called the *Softmax function*.



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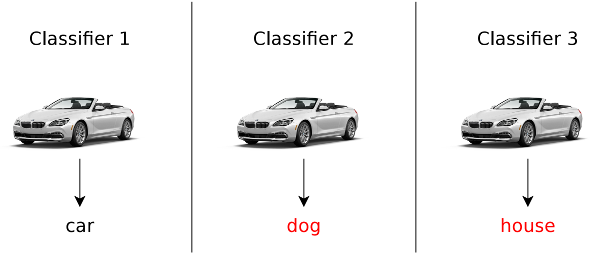
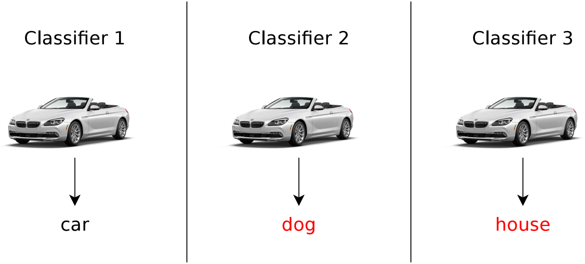
    - How about this case? Which is worse?



Loss Function



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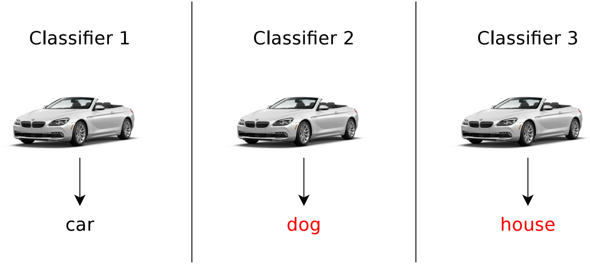

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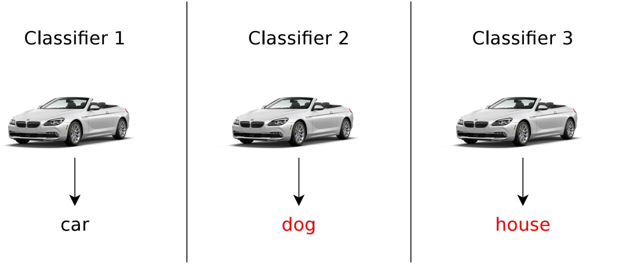

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  - How "off" is $\mathbf{y}$ from $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x};\theta)$

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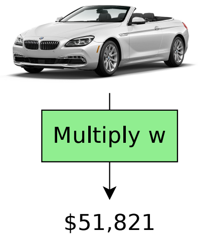

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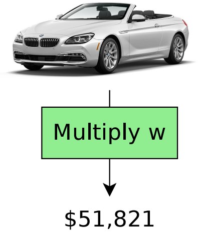

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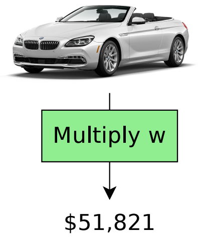
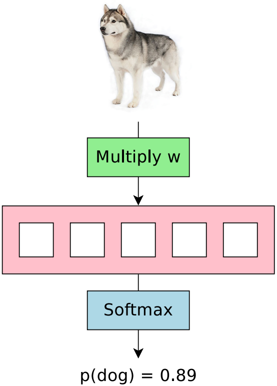
  - $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = |\hat{\mathbf{y}} - \mathbf{y}|$ is called the ℓ_1-*loss*



Case Study 2: Image classification

- Data: $\mathbf{x} \in \mathbb{R}^{3\times32\times32}$
- 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: $\theta = \{\mathbf{w} \in \mathbb{R}^{3072\times10}\}$.
  - $\mathbf{x}_1 = \text{reshape}(\mathbf{x}, [1, 3072])$
  - $\ell = \mathbf{x}_1 \cdot \mathbf{w}$
  - $\hat{p} = \textbf{Prob}\left[\mathbf{y} = i\right] = \dfrac{\exp\{\ell_i\}}{\sum_{j=1}^{5} \exp\{\ell_j\}}$



Case Study 2: Image classification

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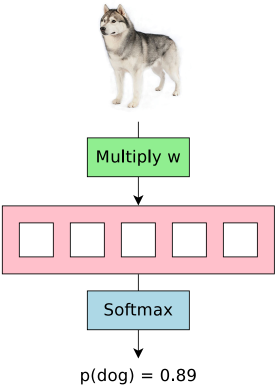

Cross-Entropy Loss

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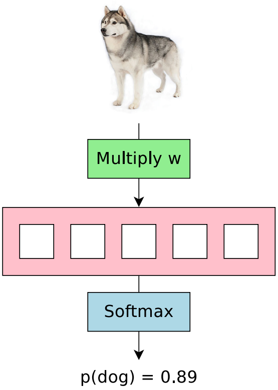

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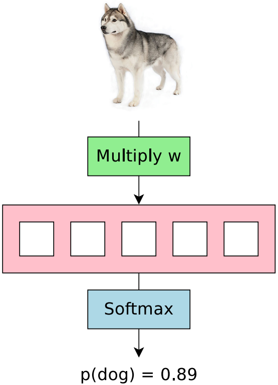

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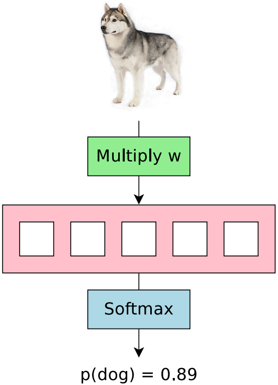

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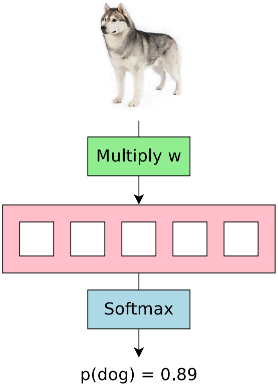

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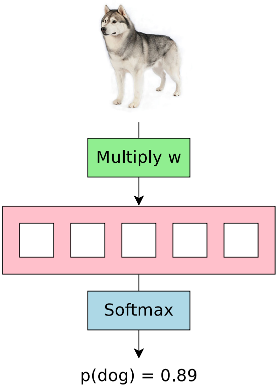
  - When $\hat{p}_{\mathbf{y}}$ is large, $\hat{p}_{\neq \mathbf{y}}$ are small
  - Differentiable. Recall $\hat{p}_i = \exp\{\ell_i\} / \sum_j \exp\{\ell_j\}$
    - ▷ Important for learning.



Outline

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The Story So Far

- **The problem:** want to learn a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$

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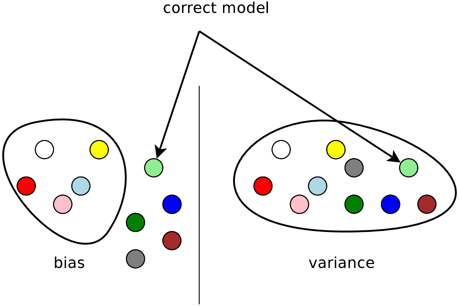

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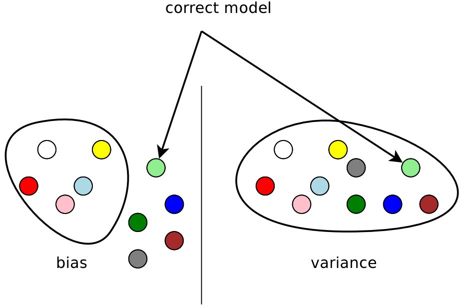
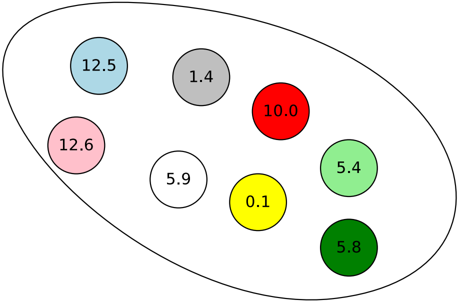


  - Come up with a *loss function* $\mathcal{L} : \mathbf{f} \in \mathcal{H} \to \mathbb{R}$, which tells you how bad is a hypothesis $\mathbf{f}$.

Learning

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



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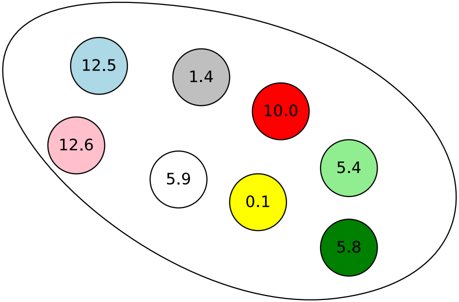

- In math: $\mathbf{f}^* = \operatorname{argmin}_{\mathbf{f} \in \mathcal{H}} \mathcal{L}(\mathbf{f})$

Case Study: Linear Regression

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- **Data:** $\{(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2), ..., (\mathbf{x}_N, \mathbf{y}_N)\}$
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Case Study: Linear Regression

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Case Study: Linear Regression

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

Case Study: Linear Regression

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

$$\ell(a, b) = \sum_{i=1}^{N} (a\mathbf{x}_i + b - \mathbf{y}_i)^2$$

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Case Study: Linear Regression

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

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

Case Study: Linear Regression

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

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

Learning is not Always Easy!

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- 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

- 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

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- 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

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- Data: $\left\{\left(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}\right), \left(\mathbf{x}^{(2)}, \mathbf{y}^{(2)}\right), ..., \left(\mathbf{x}^{(N)}, \mathbf{y}^{(N)}\right)\right\}$
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- 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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- Data: $\left\{\left(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}\right), \left(\mathbf{x}^{(2)}, \mathbf{y}^{(2)}\right), ..., \left(\mathbf{x}^{(N)}, \mathbf{y}^{(N)}\right)\right\}$
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- 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:
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- In TensorFlow: `tf.train.GradientDescentOptimizer`

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- In TensorFlow: `tf.train.GradientDescentOptimizer`
- Assuming that you have a gradient ∇_θ
- There are many other ways to update, more than just

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

Momentum

- Keeps a *running average* of ∇_θ

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

- You have to choose m, η
- In TensorFlow: `tf.train.MomentumOptimizer`

Adaptive Stochastic Gradient Descent (AdaGrad)

- Keeps a *running average* of ∇_θ^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, η
- In TensorFlow: `tf.train.AdagradOptimizer`

Outline

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1. The Learning Problem
2. Data and Label
3. Modeling
4. Error and Loss Function
5. Learning
6. Overfitting and Regularization

Is it good to minimize loss function?

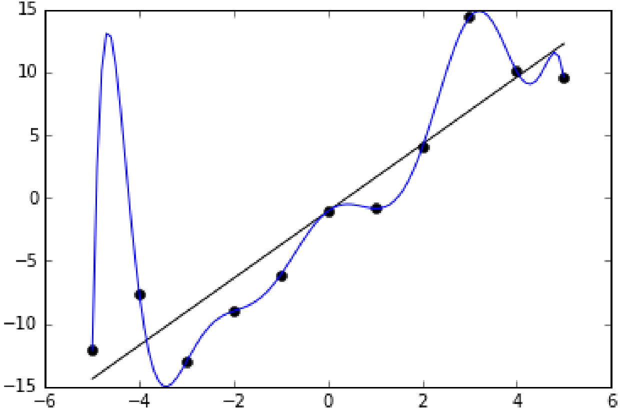

Image credit: wikipedia

Is it good to minimize loss function?

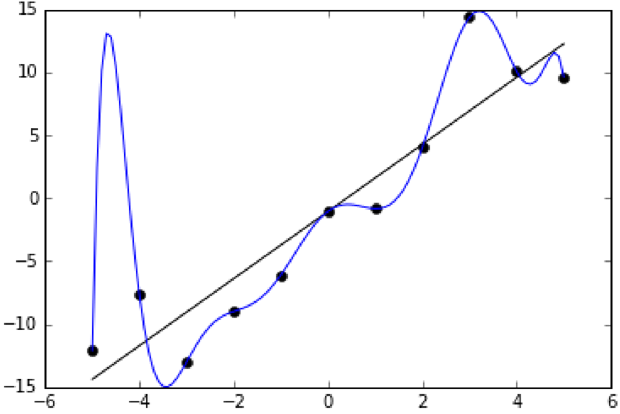

Image credit: wikipedia

- NO!

Regularization

Carnegie Mellon

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

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

- You have to choose β
- The term $\beta \left\|\theta\right\|^2$ is called the ℓ-2 regularization.

Regularization

- There are other choices
- ℓ-1 regularization

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

- ℓ-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" θ.