香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 3

Logistic Regression, Exponential Family

Junxian He
Feb 9, 2024

Classification

CAT

Labels are discrete

Logistic Regression

Logistic Regression

Given a training set $\{(x^{(i)}, y^{(i)})$ for $i = 1, \ldots, n\}$ let $y^{(i)} \in \{0, 1\}$.
Want $h_\theta(x) \in [0, 1]$. Let's pick a smooth function:

$$h_\theta(x) = g(\theta^T x)$$

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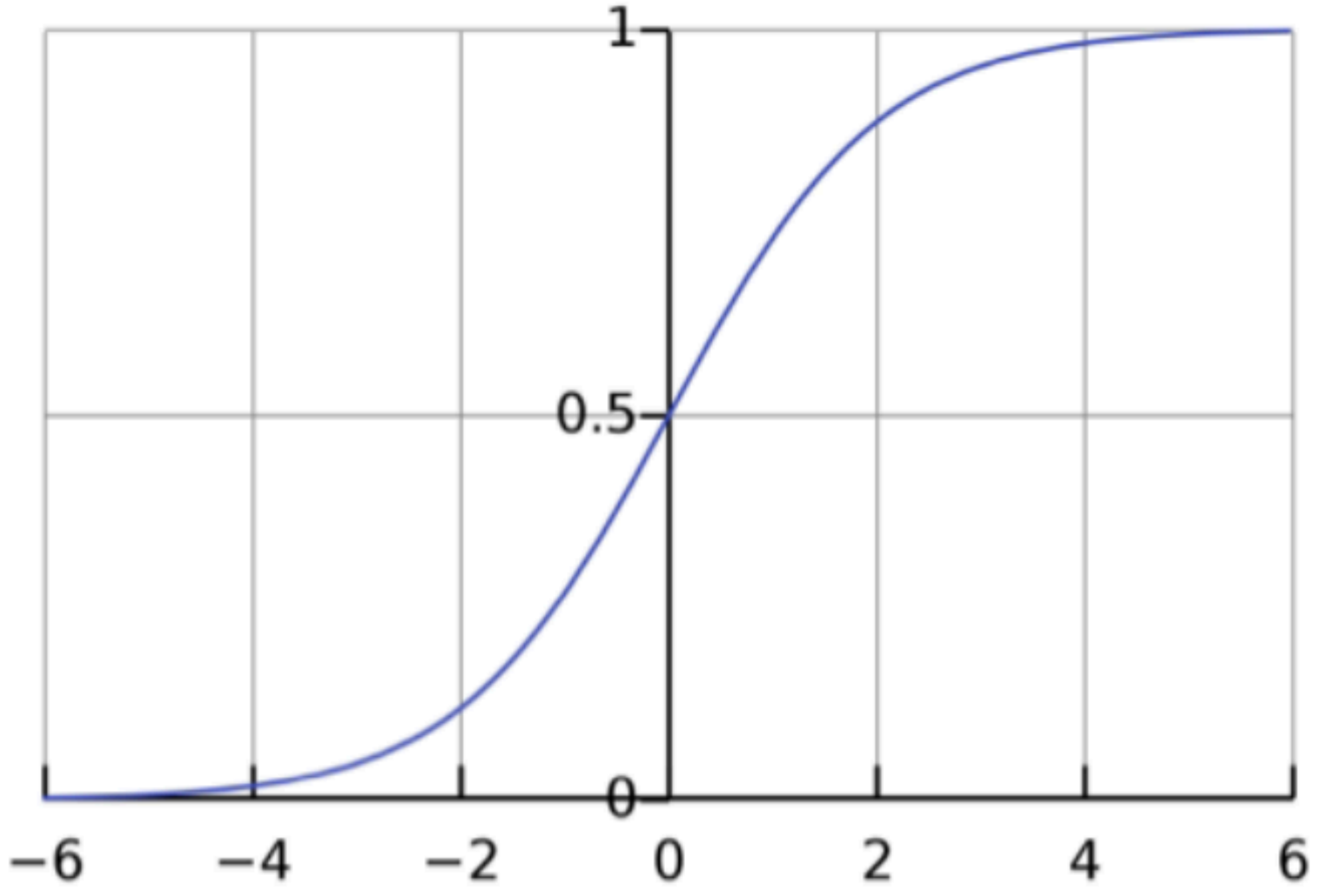

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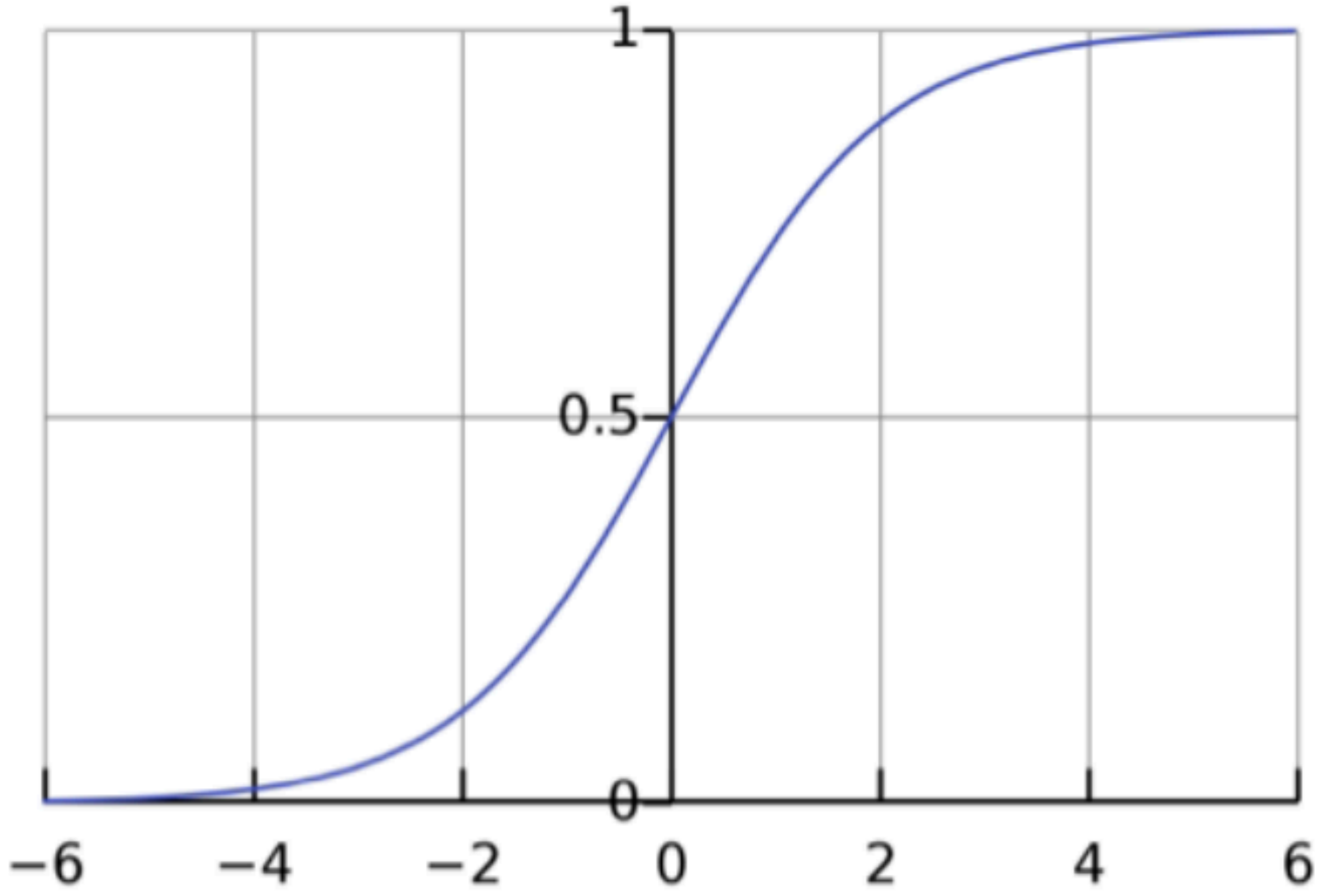

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How do we interpret $h_\theta(x)$?

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

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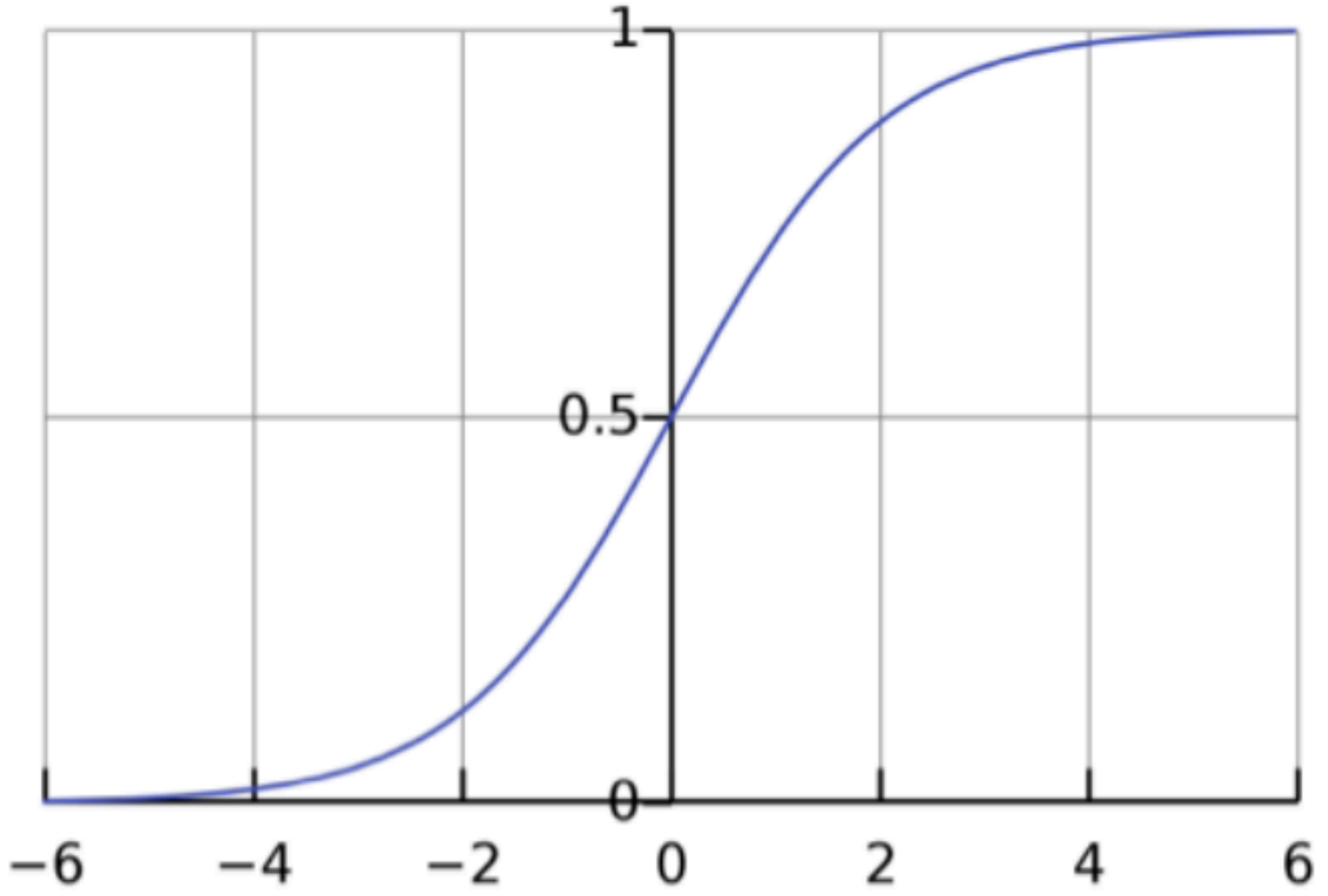

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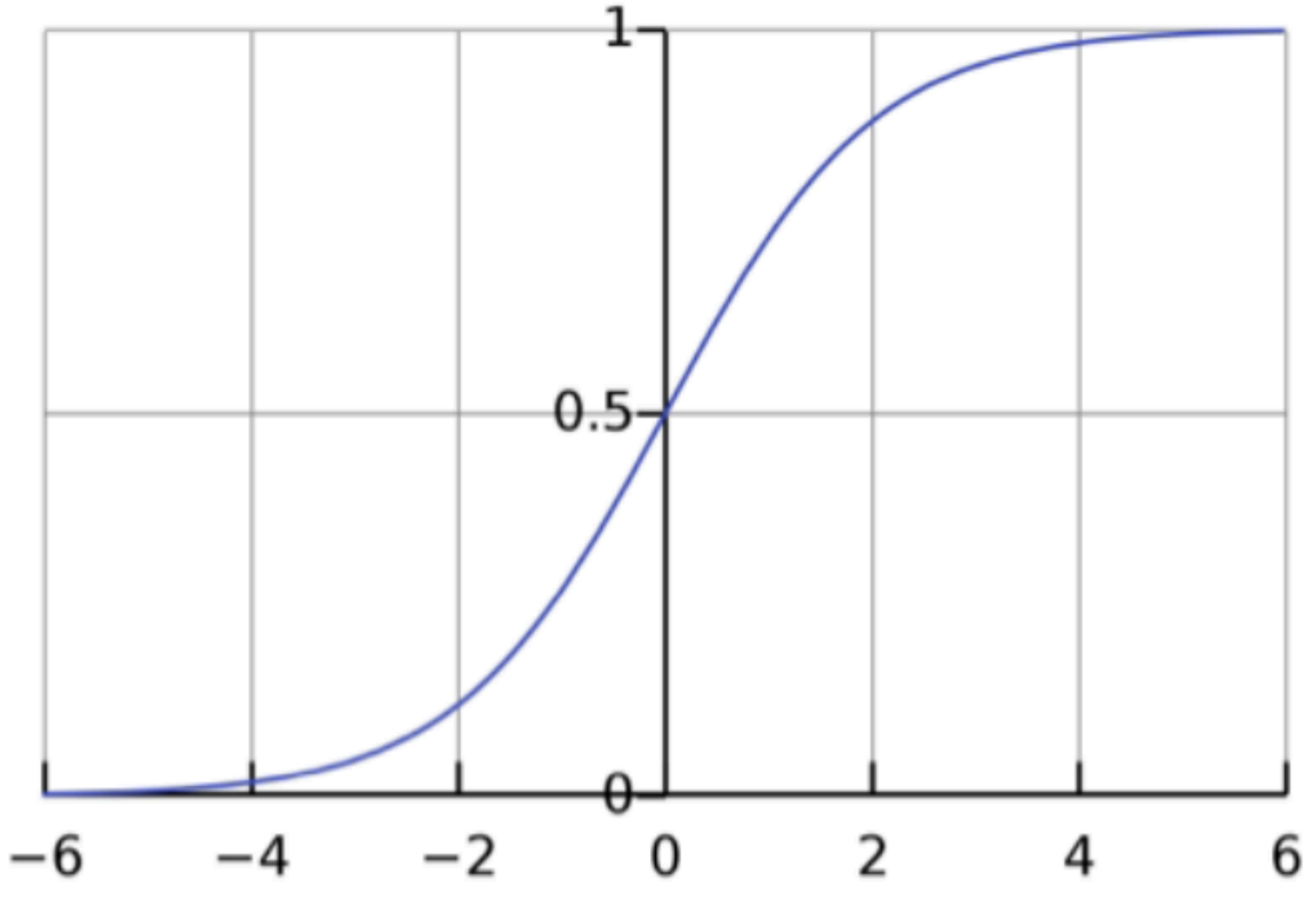

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Logistic Function

Sigmoid Function

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Logistic Regression

Let's write the Likelihood function. Recall:

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\begin{aligned}
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\end{aligned}
$$

Maximum likelihood estimation

Logistic Regression

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Then,

$$L(\theta) = P(y \mid X; \theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta)$$

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$$= \prod_{i=1}^{n} h_\theta(x^{(i)})^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}}$$

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$$= \prod_{i=1}^{n} h_\theta(x^{(i)})^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}}$$

Taking logs to compute the log likelihood $\ell(\theta)$ we have:

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

Maximum likelihood estimation

Derivative of Logistic Function

$$
\begin{aligned}
g'(z) &= \frac{d}{dz} \frac{1}{1+e^{-z}} \\
&= \frac{1}{(1+e^{-z})^2} \left(e^{-z}\right) \\
&= \frac{1}{(1+e^{-z})} \cdot \left(1 - \frac{1}{(1+e^{-z})}\right) \\
&= g(z)(1-g(z)).
\end{aligned}
$$

Gradient Descent

$$
\begin{aligned}
\frac{\partial}{\partial \theta_j} \ell(\theta) &= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1 - g(\theta^T x)} \right) \frac{\partial}{\partial \theta_j} g(\theta^T x) \\
&= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1 - g(\theta^T x)} \right) g(\theta^T x)(1 - g(\theta^T x)) \frac{\partial}{\partial \theta_j} \theta^T x \\
&= \left(y(1 - g(\theta^T x)) - (1-y) g(\theta^T x) \right) x_j \\
&= (y - h_\theta(x)) \, x_j
\end{aligned}
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\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}
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Looks identical to LMS update rule in linear regression

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Looks identical to LMS update rule in linear regression

Is this coincidence?

Multi-Label Classification

{Cat, dog, dragon, fish, pig}

Multi-Label Classification

Given a training set $\{(x^{(1)}, y^{(1)}), \cdots, (x^{(n)}, y^{(n)})\}, y^{(i)} \in \{1,2,\cdots,k\}$,
we aim to model the distribution $p(y \mid x; \theta)$

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Categorical distribution, $p(y = k \mid x; \theta) = \phi_k$

s.t. $\sum_{i=1}^{k} \phi_i = 1$

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$\phi_i = \theta_i^T x$?

Softmax Function

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Softmax: $\mathbb{R}^k \rightarrow \mathbb{R}^k$

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$$\text{softmax}(t_1, \ldots, t_k) = \begin{bmatrix} \frac{\exp(t_1)}{\sum_{j=1}^{k} \exp(t_j)} \\ \vdots \\ \frac{\exp(t_k)}{\sum_{j=1}^{k} \exp(t_j)} \end{bmatrix}$$

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The denominator is a normalization constant

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$$\text{Let } (t_1, \ldots, t_k) = (\theta_1^\top x, \cdots, \theta_k^\top x)$$

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Chain rule

$$\frac{\partial \ell_{\text{ce}}((\theta_1^\top x, \ldots, \theta_k^\top x), y)}{\partial \theta_i} = \frac{\partial \ell(t,y)}{\partial t_i} \cdot \frac{\partial t_i}{\partial \theta_i} = (\phi_i - 1\{y=i\}) \cdot x$$

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$$\frac{\partial \ell(\theta)}{\partial \theta_i} = \sum_{j=1}^{n}(\phi_i^{(j)} - 1\{y^{(j)}=i\})\cdot x^{(j)}$$

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$$\frac{\partial \ell(\theta)}{\partial \theta_i} = \sum_{j=1}^{n} (\phi_i^{(j)} - 1\{y^{(j)} = i\}) \cdot x^{(j)}$$

Intuitive explanation of the rule?

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- This is the update rule in 1d

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$$\downarrow$$

Solution to a linear equation

$$f'(x^{(t)})x^{(t+1)} + f(x^{(t)}) - x^{(t)}f'(x^{(t)}) = 0$$

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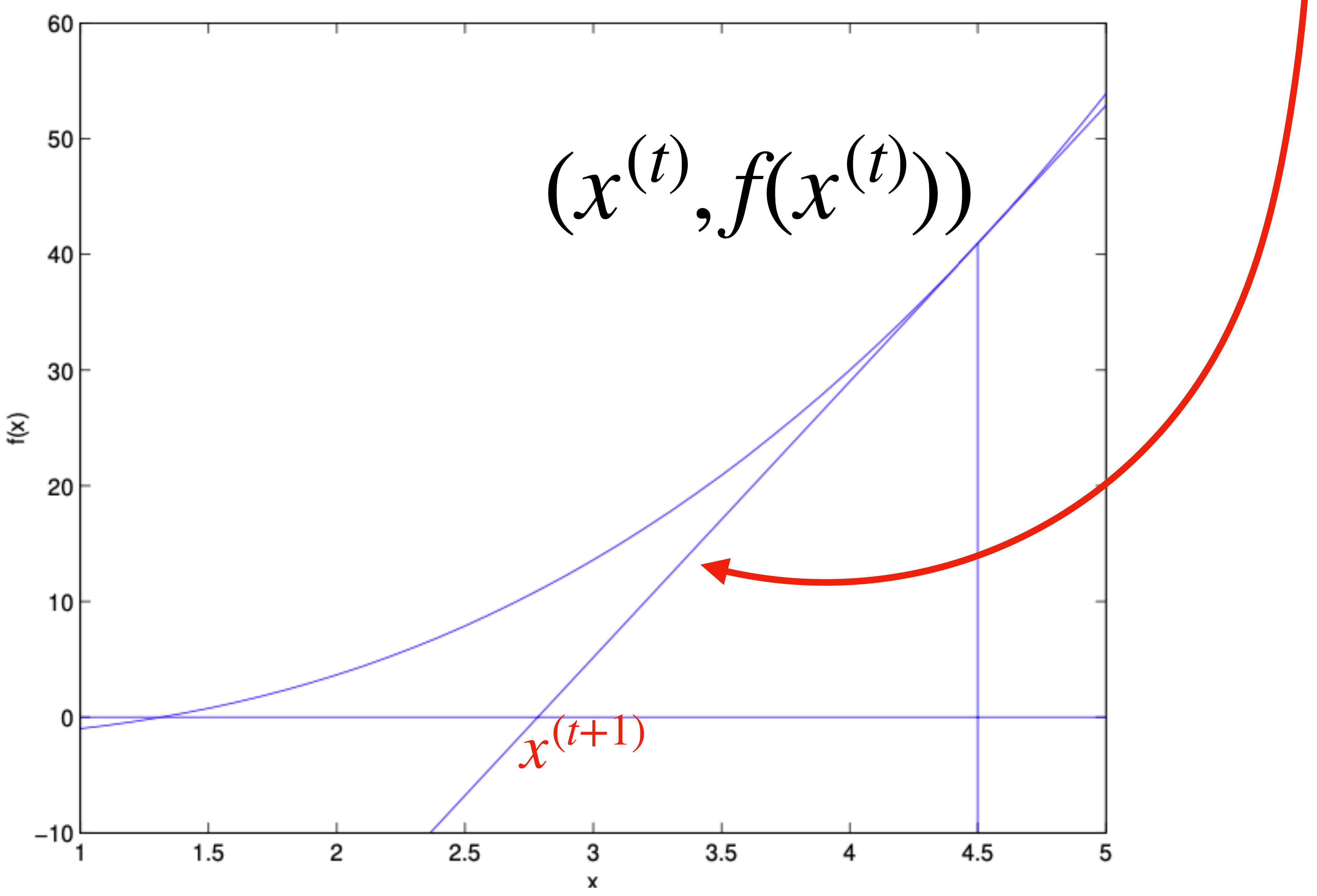
$\downarrow$ Solution to a linear equation

$$f'(x^{(t)})x^{(t+1)} + f(x^{(t)}) - x^{(t)}f'(x^{(t)}) = 0$$

View it as a equation of $x^{(t+1)}$, and $x^{(t)}$ is a constant

Another Optimization Method — Newton's Method

$$f'(x^{(t)})x + f(x^{(t)}) - x^{(t)}f'(x^{(t)}) = y$$



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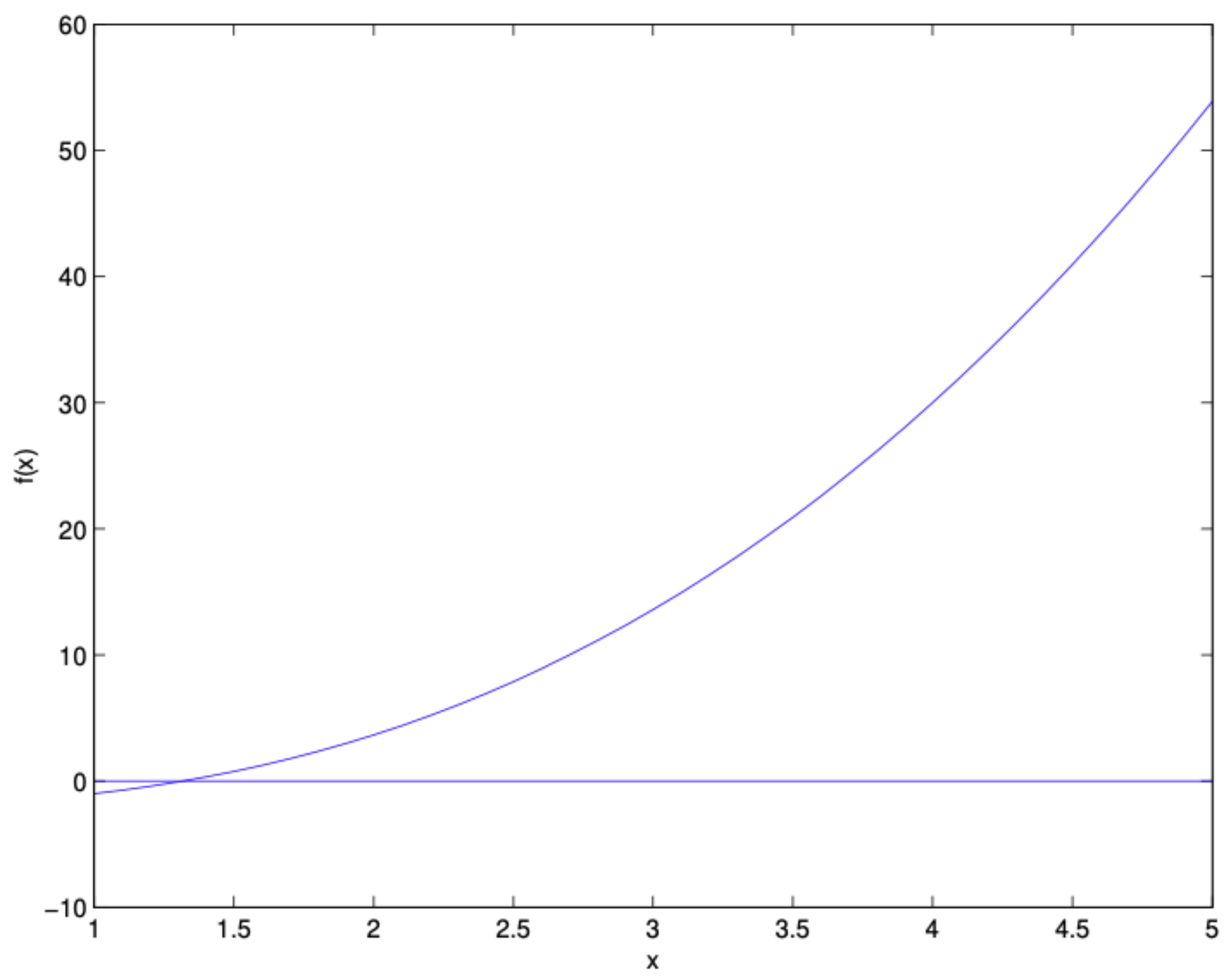

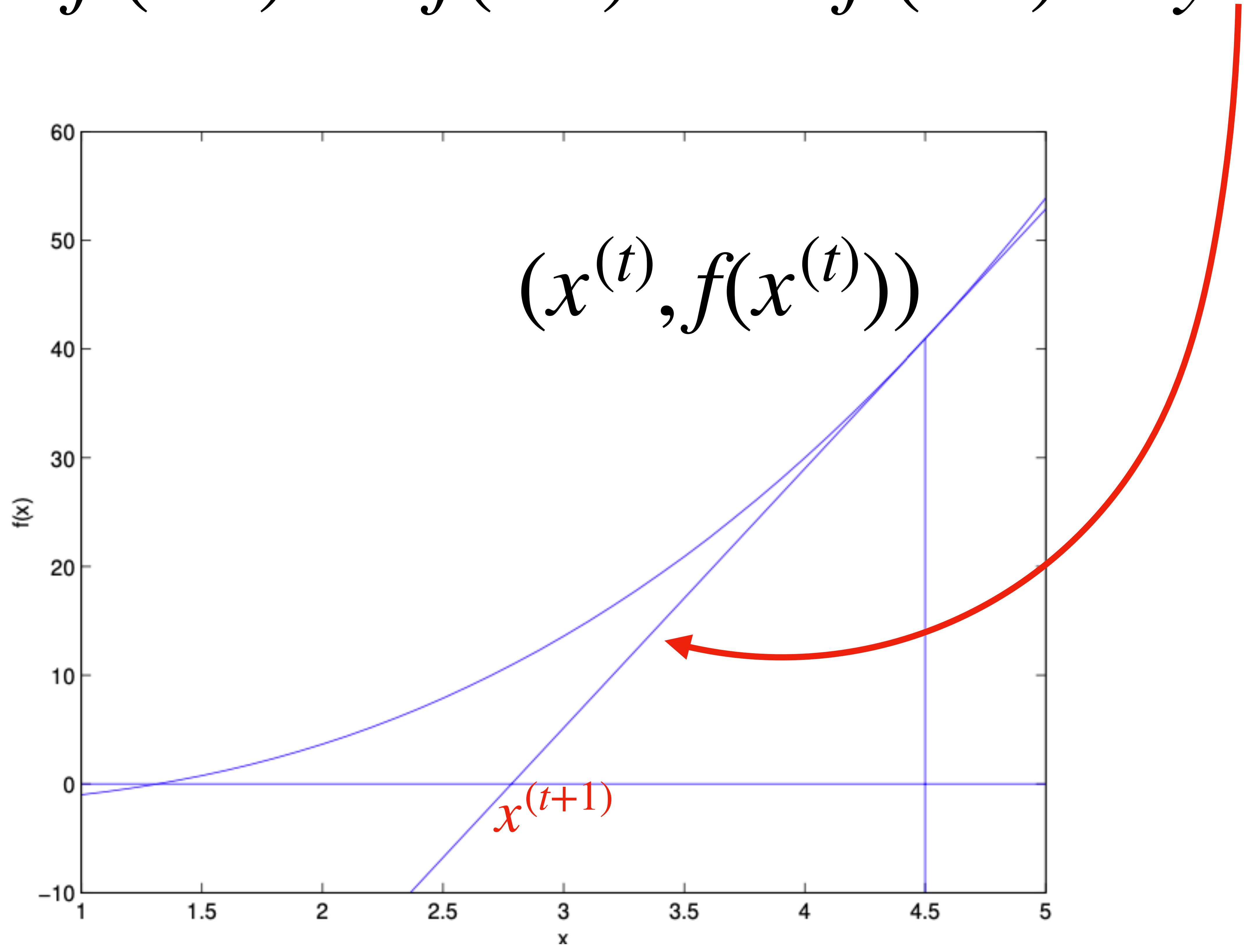

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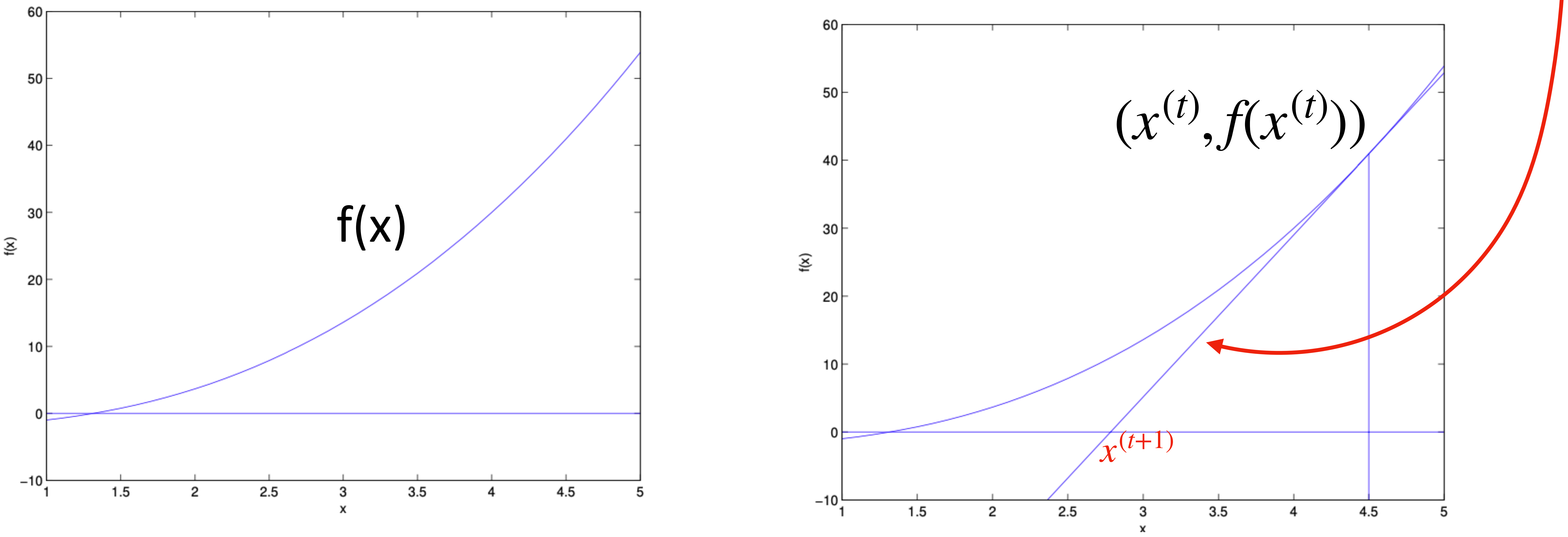

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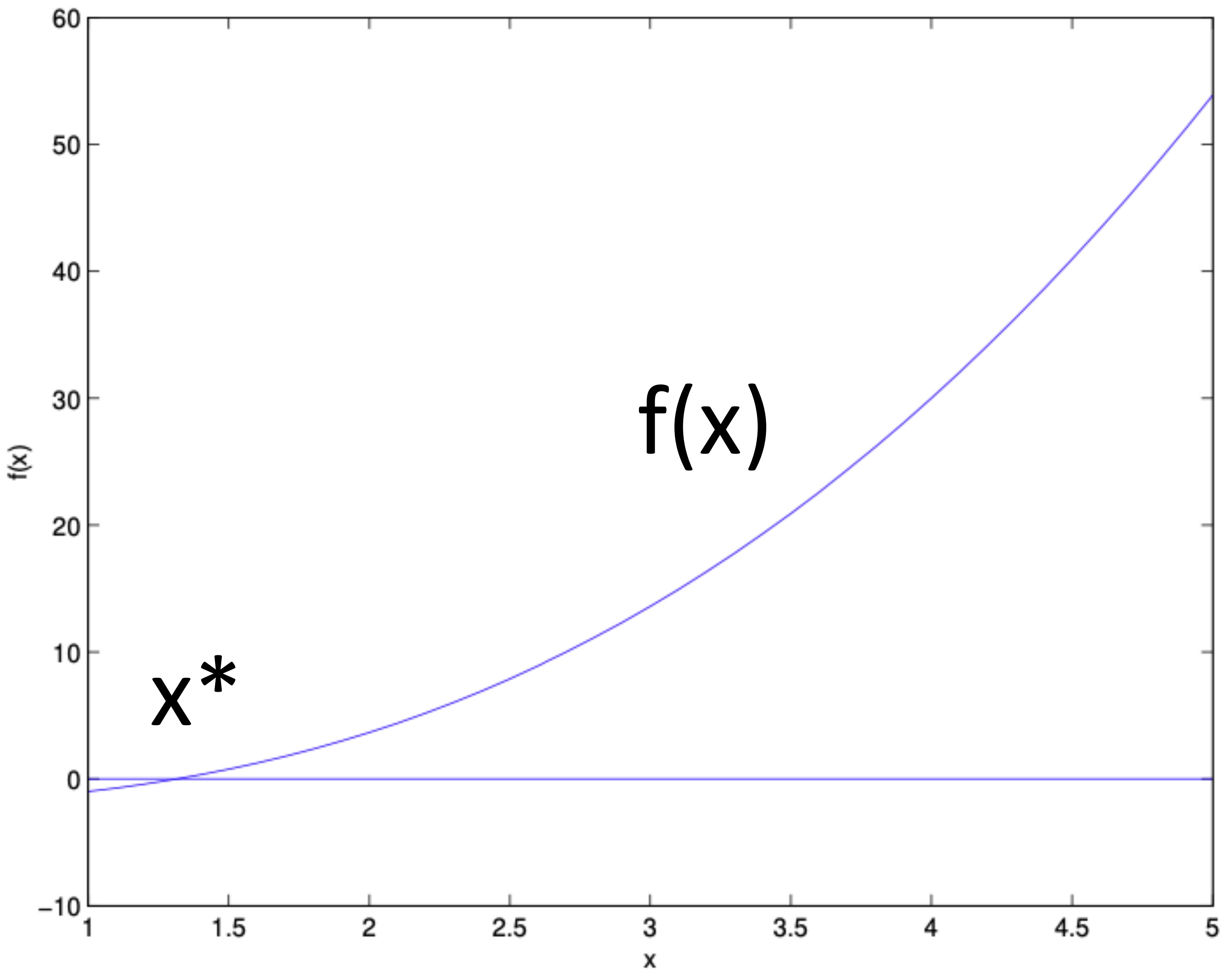

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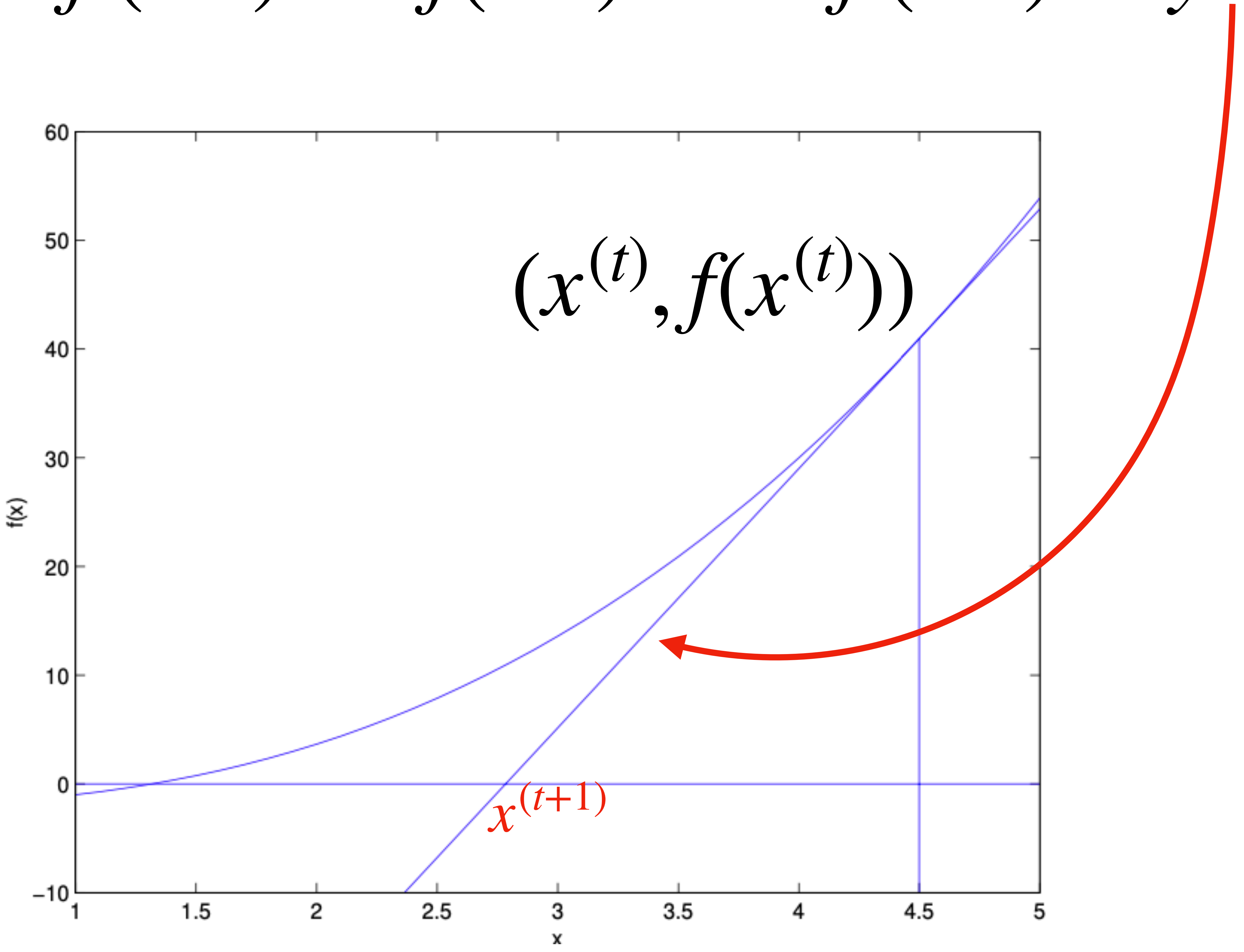

Another Optimization Method — Newton's Method

Given $f : \mathbb{R}^d \to \mathbb{R}$ find x s.t. $f(x) = 0$. $\nabla_\theta l(\theta) = 0$

- This is the update rule in 1d

$$x^{(t+1)} = x^{(t)} - \frac{f(x^{(t)})}{f'(x^{(t)})} \qquad \theta := \theta - \frac{\ell'(\theta)}{\ell''(\theta)}.$$

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- For the likelihood, i.e., $f(\theta) = \nabla_\theta \ell(\theta)$ we need to generalize to a vector-valued function which has:

$$\theta^{(t+1)} = \theta^{(t)} - \left(H(\theta^{(t)})\right)^{-1} \nabla_\theta \ell(\theta^{(t)}).$$

in which $H_{i,j}(\theta) = \frac{\partial}{\partial\theta_i \partial\theta_j} \ell(\theta)$.

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$$x^{(t+1)} = x^{(t)} - \frac{f(x^{(t)})}{f'(x^{(t)})} \qquad \theta := \theta - \frac{\ell'(\theta)}{\ell''(\theta)}.$$

- It may converge *very* fast (quadratic local convergence!) Requires fewer iterations
- For the likelihood, i.e., $f(\theta) = \nabla_\theta \ell(\theta)$ we need to generalize to a vector-valued function which has:

$$\theta^{(t+1)} = \theta^{(t)} - \left(H(\theta^{(t)})\right)^{-1} \nabla_\theta \ell(\theta^{(t)}).$$

in which $H_{i,j}(\theta) = \frac{\partial}{\partial\theta_i \partial\theta_j} \ell(\theta)$.

When Newton's method is applied to maximize the logistic regression log likelihood function l(θ), the resulting method is also called Fisher scoring.

Exponential Family

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- Exponential family unifies inference and learning for many important models

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Rough Idea *"If P has a a special form, then inference and learning come for free"*

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Here y, $a(\eta)$, and $b(y)$ are scalars. $T(y)$ same dimension as η.

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$$1 = \sum_y P(y;\eta) = e^{-a(\eta)} \sum_y b(y) \exp\left\{\eta^T T(y)\right\}$$

$$\implies a(\eta) = \log \sum_y b(y) \exp\left\{\eta^T T(y)\right\}$$

Example: Bernoulli

Bernoulli random variable is an event (say flipping a coin) then:

$$p(y; \phi) = \phi^y (1 - \phi)^{1-y}$$

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We need to show $a(\eta)$ is a function of $\log\frac{\phi}{1-\phi}$

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We first observe that:

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We have verified Bernoulli distribution is in the exponential family

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Is this true for general?

Log Partition Function

Yes! Recall that

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Then, taking derivatives

$$\nabla_\eta a(\eta) = \frac{\sum_y T(y) b(y) \exp\{\eta^T T(y)\}}{\sum_y b(y) \exp\{\eta^T T(y)\}} = \mathbb{E}[T(y); \eta]$$

Many Other Exponential Models

- There are many canonical exponential family models:
  - Binary $\mapsto$ Bernoulli
  - Multiple Classses $\mapsto$ Multinomial
  - Real $\mapsto$ Gaussian
  - Counts $\mapsto$ Poisson
  - $\mathbb{R}_+ \mapsto$ Gamma, Exponential
  - Distributions $\mapsto$ Dirichlet

Thank You!
Q & A