Deep Learning & Applied AI

Overfitting and going nonlinear

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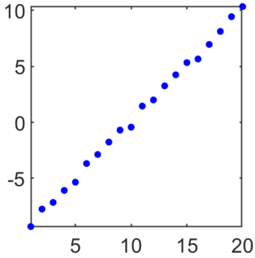
A glimpse into neural networks

In deep learning, we deal with highly parametrized models called deep neural networks:

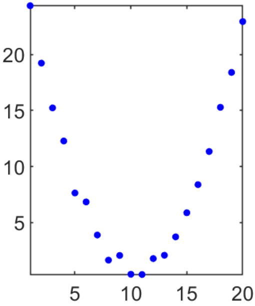
$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

Parametrized models

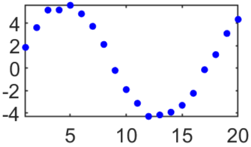
The parameters describe the behavior of the network, and must be solved for.



$y = ax + b$



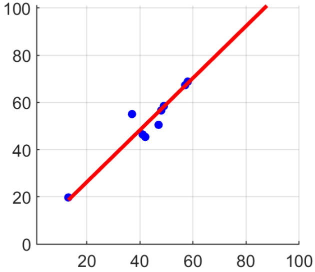
$y = ax^2 + bx + c$



$y = a\sin(x) + bx + c$

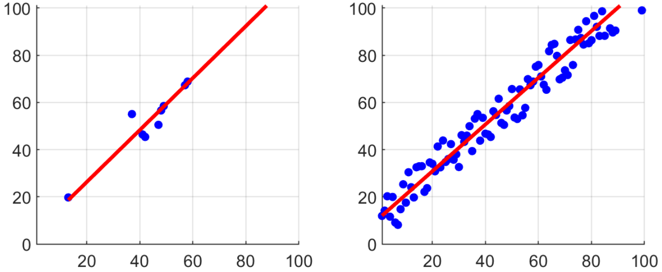
From a technical standpoint, our task is to determine the parameters Θ.

Data distribution



Assumption: linear model

Data distribution



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More data allows us to improve our prediction

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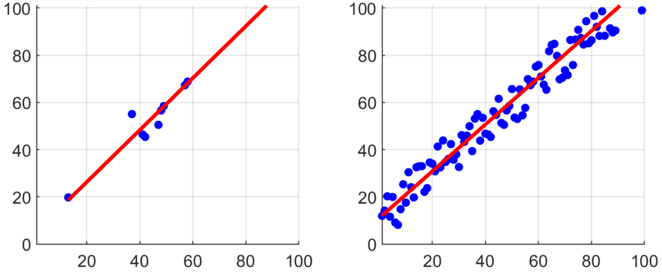

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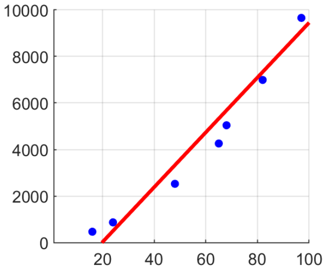
What if the assumption (i.e. linear prior here) is **wrong**?

Data distribution



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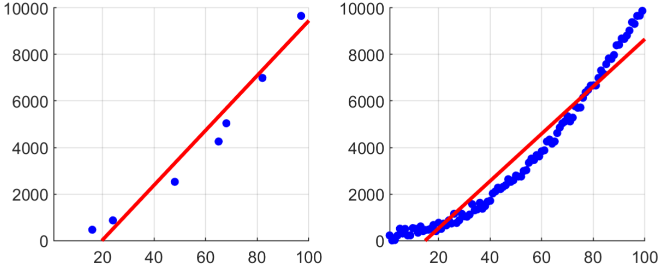
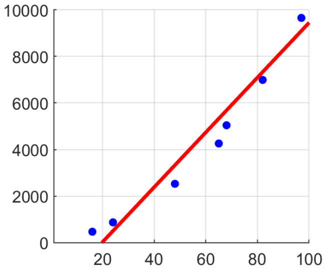
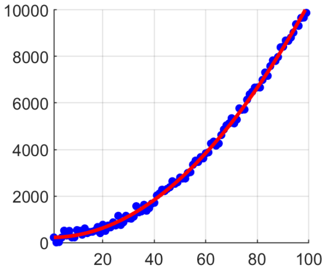


Assumption: linear model

More data confutes our assumptions

Data distribution





Assumption: quadratic model

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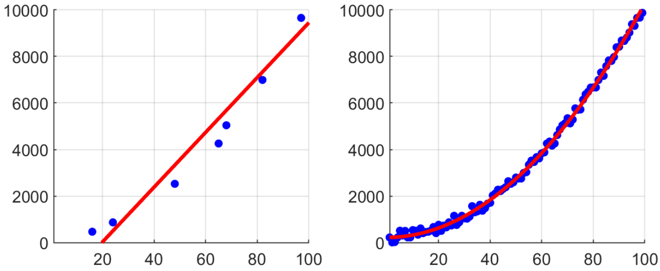

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Key questions:

- How to select the correct distribution?

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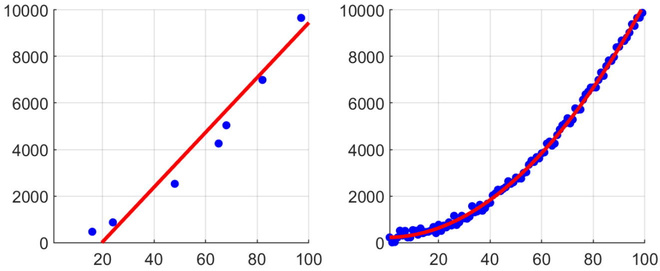

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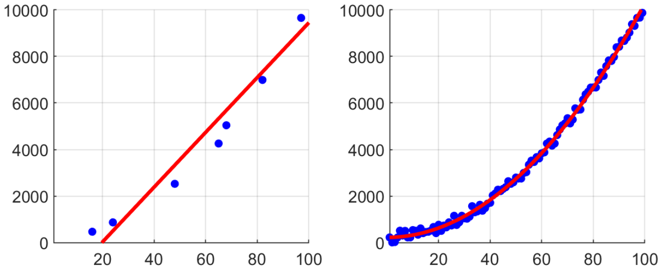


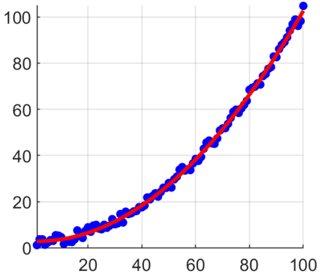
Assumption: quadratic model

Key questions:

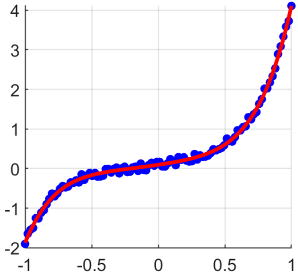
- How to select the correct distribution?
- How much data do we need?
- What if the correct distribution does not admit a simple expression?

Polynomial regression

After the linear model, the simplest thing is a polynomial model.



2nd-order



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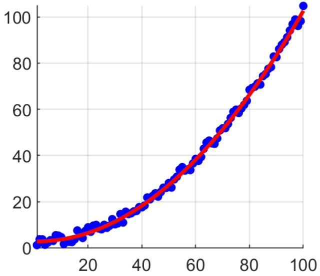

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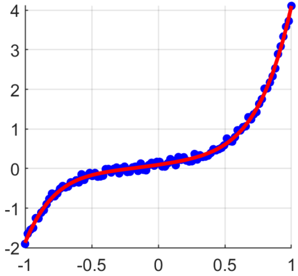

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The number of parameters grows with the order.

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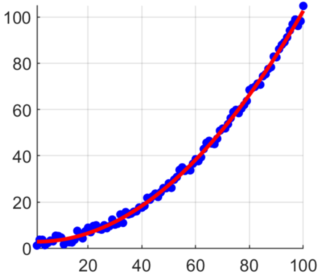

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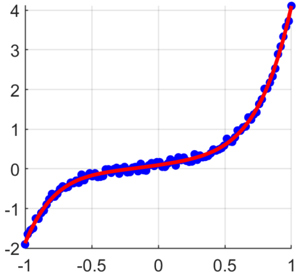

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The number of parameters grows with the order.

More data are needed to make an informed decision on the order.

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In matrix notation:

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} x_1^k & x_1^{k-1} & \cdots & x_1 & 1 \\ x_2^k & x_2^{k-1} & \cdots & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^k & x_n^{k-1} & \cdots & x_n & 1 \end{pmatrix}}_{\mathbf{X}} \underbrace{\begin{pmatrix} a_k \\ a_{k-1} \\ \vdots \\ a_1 \\ b \end{pmatrix}}_{\boldsymbol{\theta}}$$

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The same exact least-squares solution as with linear regression applies, with the requirement that $k < n$.

Polynomial fitting

An application of the Stone-Weierstrass theorem tells us:

If f is continuous on the interval $[a, b]$, then for every $\epsilon > 0$ there exists a polynomial p such that $|f(x) - p(x)| < \epsilon$ for all x.

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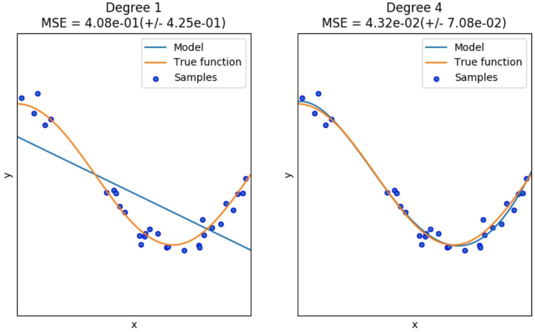

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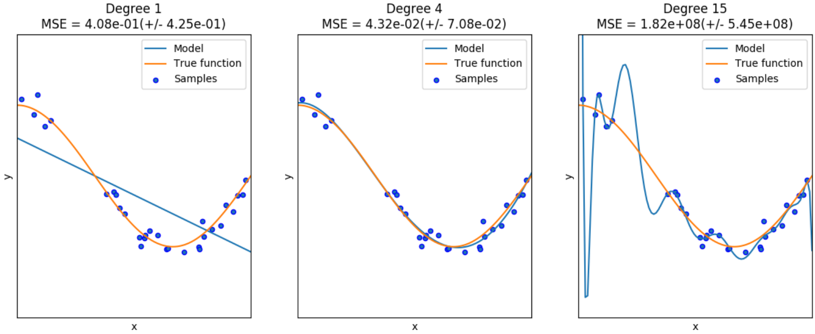

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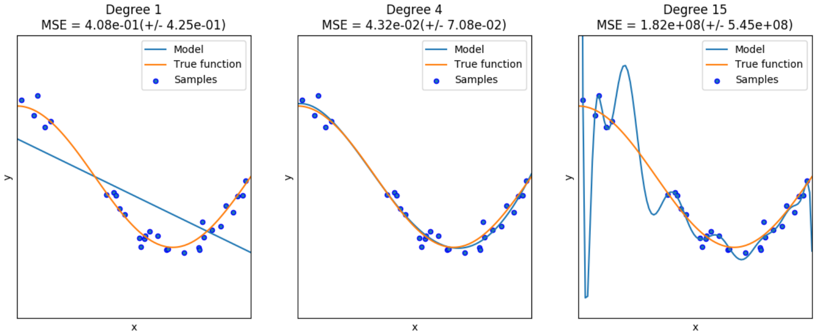

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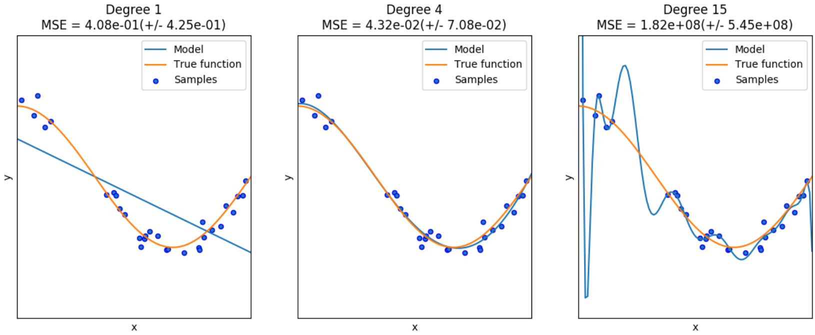

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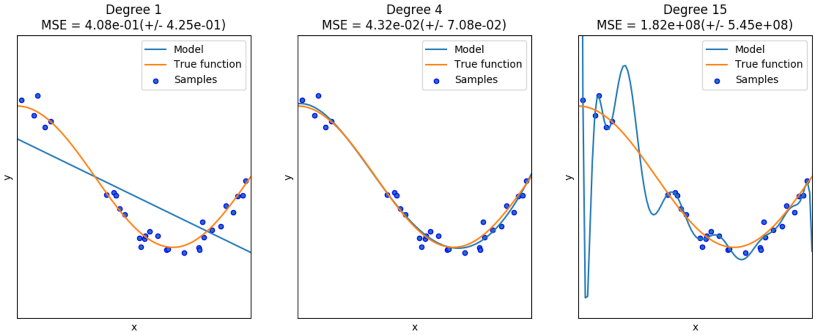

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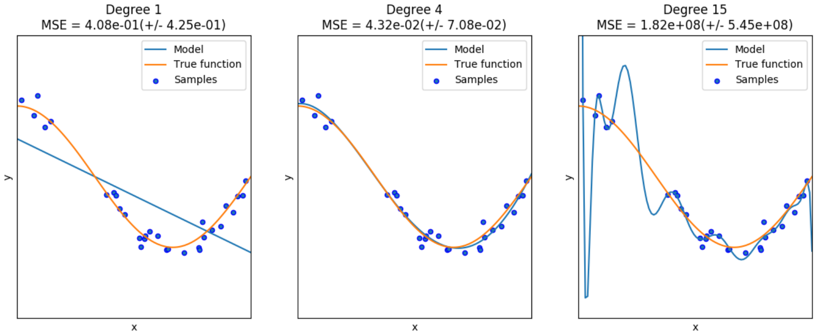

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Adding complexity can lead to overfitting and thus worse generalization.

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4. Large MSE on the validation $\Rightarrow$ overfitting $\Rightarrow$ bad generalization

Underfitting:
large training error, large validation error

Underfitting vs. Overfitting

Underfitting:
large training error, large validation error

Overfitting:
(very) small training error, large validation error

Not done yet

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- Different loss than MSE
- Regularization
- Additional priors
- Intermediate features
- Flexibility
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From now on, we embrace the idea that many natural phenomena of interest are nonlinear.

Regularization penalties

Sometimes our prior knowledge can be expressed in terms of an energy.

For example, avoid large parameters to counteract overfitting:

$$\min_{\boldsymbol{\Theta}} \underbrace{\ell_{\boldsymbol{\Theta}}}_{\text{data term}} + \underbrace{\lambda}_{\text{trade-off}} \cdot \underbrace{\|\Theta\|_F^2}_{\text{regularizer}}$$

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More in general:

$$\min_{\mathbf{\Theta}} \ell_{\mathbf{\Theta}} + \lambda \|\Theta\|_p$$

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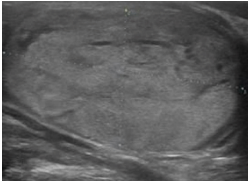
Classification

What if we want to predict a category instead of a value?

$$f_\Theta(\quad$$



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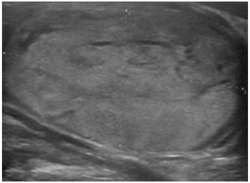
$f_{\Theta}($  $) = \{0, 1\}$

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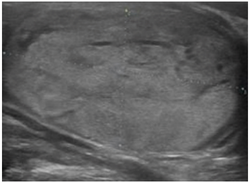

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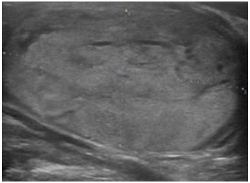
$f_\Theta($  $) = \{0, 1\}$

Possible solution: Do post-processing (e.g. thresholding) to convert linear regression to a binary output.

$\Rightarrow$ The solution is not necessarily an optimum anymore.

Instead: Modify the loss to minimize over categorical values directly.

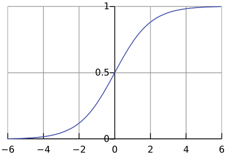
Logistic regression

New loss:

$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} (y_i - \sigma(\underbrace{ax_i + b}_{\text{linear}}))^2$$

Here, σ is the nonlinear logistic sigmoid:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



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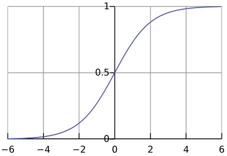

σ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

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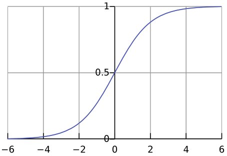

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$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} c(x_i, y_i)\,, \quad \text{with}$$

$$c(x_i, y_i) = \begin{cases} -\ln(\sigma(ax_i + b)) & y_i = 1 \\ -\ln(1 - \sigma(ax_i + b)) & y_i = 0 \end{cases} \qquad \text{convex}$$

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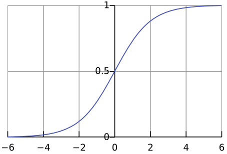

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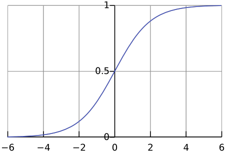

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Logistic regression

New convex loss:

$$\ell_\Theta(\{x_i, y_i\}) = -\sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i)\ln(1 - \sigma(ax_i + b))$$

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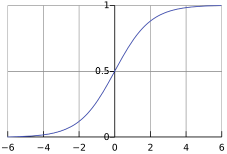
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



σ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_{\Theta} \ell_{\Theta} = 0$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i)\ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$\nabla_\Theta \left(y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) \right)$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

$$\nabla_\Theta \sum_{i=1}^{n} y_i \ln(\sigma(ax_i + b)) + (1 - y_i) \ln(1 - \sigma(ax_i + b)) = 0$$

where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$\nabla_\Theta y_i \ln(\sigma(ax_i + b)) + \nabla_\Theta (1 - y_i) \ln(1 - \sigma(ax_i + b))$$

Logistic regression: Finding a solution

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where $\Theta = \{a, b\}$.

Consider the gradient of each term in the summation:

$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Logistic regression: Finding a solution

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$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial a}$$

Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial}{\partial a} a x_i + b$$

Logistic regression: Finding a solution

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$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial \sigma(ax_i + b)}{\partial (ax_i + b)} \cdot x_i$$

Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{\partial}{\partial(ax_i + b)} \frac{1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{e^{-(ax_i + b)}}{(1 + e^{-(ax_i + b)})^2} \cdot x_i$$

Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i+b)}} \frac{e^{-(ax_i+b)}}{1 + e^{-(ax_i+b)}} \cdot x_i$$

Logistic regression: Finding a solution

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} \frac{(1 + e^{-(ax_i + b)}) - 1}{1 + e^{-(ax_i + b)}} \cdot x_i$$

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$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \frac{1}{1 + e^{-(ax_i + b)}} (1 - \frac{1}{1 + e^{-(ax_i + b)}}) \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial f}{\partial g} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

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Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{\partial \ln(\sigma(ax_i + b))}{\partial \sigma(ax_i + b)} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

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$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} f(g(h(a, b))) = \frac{1}{\sigma(ax_i + b)} \cdot \sigma(ax_i + b)(1 - \sigma(ax_i + b)) \cdot x_i$$

Logistic regression: Finding a solution

Since the loss is convex, the first-order conditions apply:

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$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i) \nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b)) x_i$$

Logistic regression: Finding a solution

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$$y_i \nabla_\Theta \underbrace{\ln(\sigma(ax_i + b))}_{f(g(h(\Theta)))} + (1 - y_i)\nabla_\Theta \ln(1 - \sigma(ax_i + b))$$

Apply the chain rule to each partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

And similarly for the second term and for parameter b.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a}\ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.

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- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

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model	**loss**	**solution**
linear regression		
linear regression + Tikhonov		
logistic regression		

Logistic regression: Finding a solution

By looking at the partial derivative:

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model	**loss**	**solution**
linear regression	convex	
linear regression + Tikhonov	convex	
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.
- $\nabla \ell_\Theta = 0$ is a transcendental equation $\Rightarrow$ no analytical solution.

model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(ax_i + b)) = (1 - \sigma(ax_i + b))x_i$$

we see that the parameters enter the gradient in a nonlinear way.

Thus:

- $\nabla \ell_\Theta = 0$ is not a linear system that we can solve easily.
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model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	

Logistic regression: Finding a solution

By looking at the partial derivative:

$$\frac{\partial}{\partial a} \ln(\sigma(a x_i + b)) = (1 - \sigma(a x_i + b)) x_i$$

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model	**loss**	**solution**
linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	nonlinear optimization

Suggested reading

On polynomial regression vs. neural nets:
https://arxiv.org/pdf/1806.06850

Proof that the logistic loss is convex:
https://math.stackexchange.com/questions/1582452/logistic-regression-prove-that-the-cost-function-is-convex