Deep Learning & Applied AI

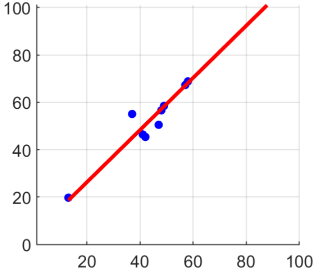
Overfitting and going nonlinear

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

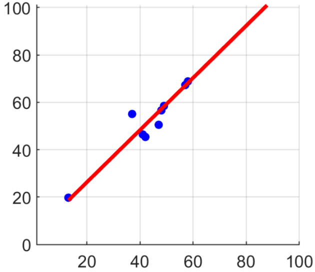
2nd semester a.y. 2023/2024 · March 11, 2024

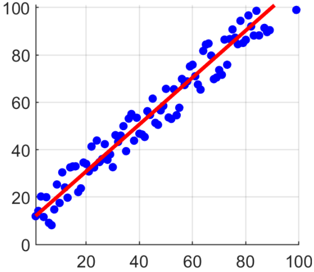
Data distribution



Assumption: linear model

Data distribution

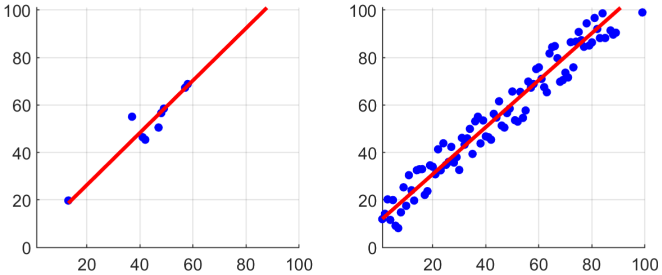




Assumption: linear model

More data allows us to improve our prediction

Data distribution

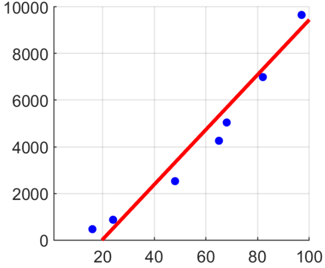


Assumption: linear model

More data allows us to improve our prediction

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

Data distribution



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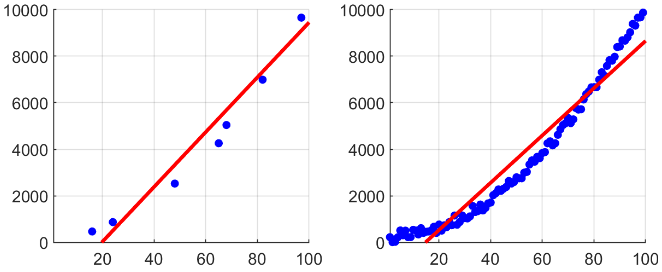
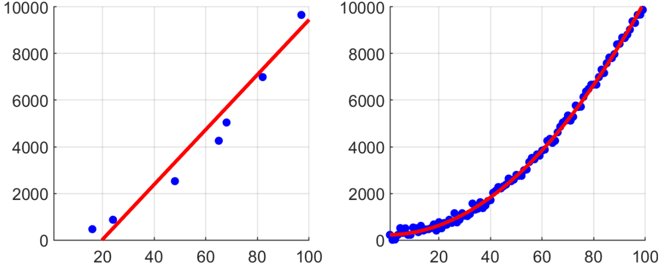


Assumption: linear model

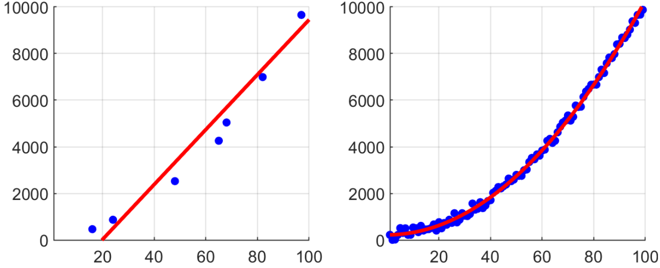
More data confutes our assumptions

Data distribution



Assumption: quadratic model

Data distribution

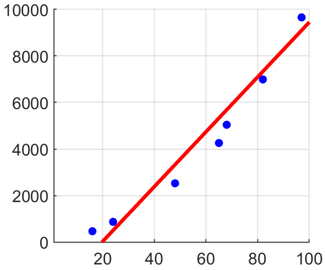


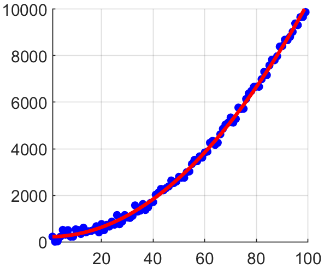
Assumption: quadratic model

Key questions:

- How to select the correct distribution?

Data distribution





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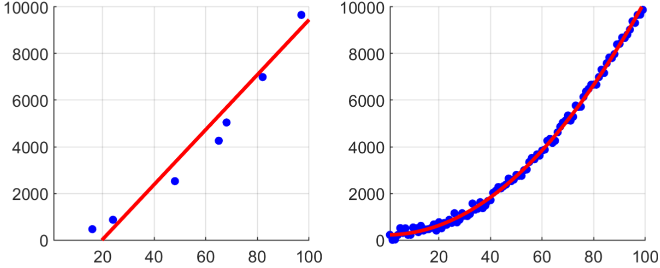
Key questions:

- How to select the correct distribution?
- How much data do we need?

Data distribution



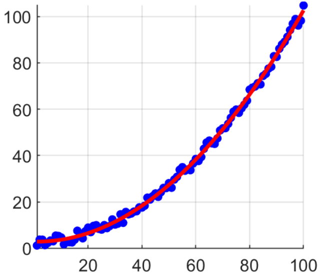
Assumption: quadratic model

Key questions:

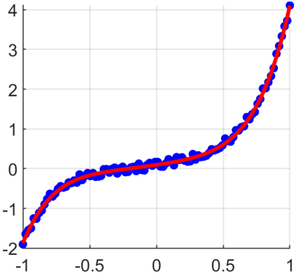
- How to select the correct distribution?
- How much data do we need?
- What if the correct distribution does not admit a simple expression?

Polynomial regression

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



2nd-order



5th-order

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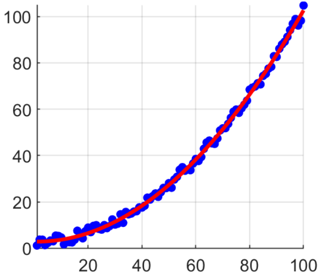

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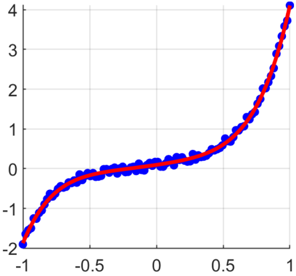

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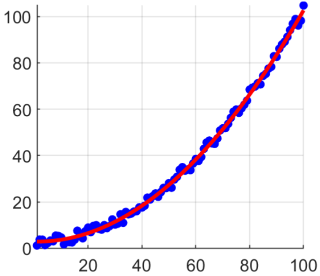

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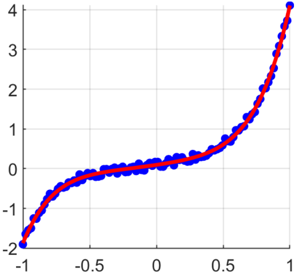

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The number of parameters grows with the order.

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

Polynomial regression

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Linear regression with polynomial features

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$$y_i = a_3 x_i^3 + a_2 x_i^2 + a_1 x_i + b \quad \text{for all data points } i = 1, \ldots, n$$

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$$y_i = b + \sum_{j=1}^{k} a_j x_i^j \quad \text{for all data points } i = 1, \ldots, n$$

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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 $|f(x) - p(x)| < \epsilon \ \forall x$.

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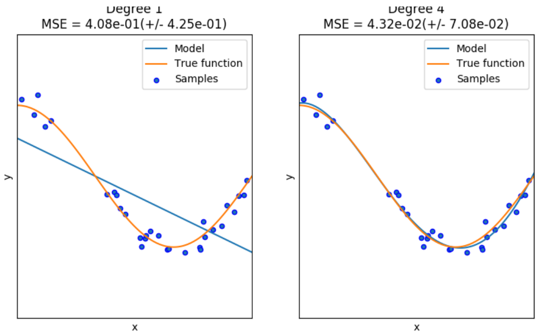

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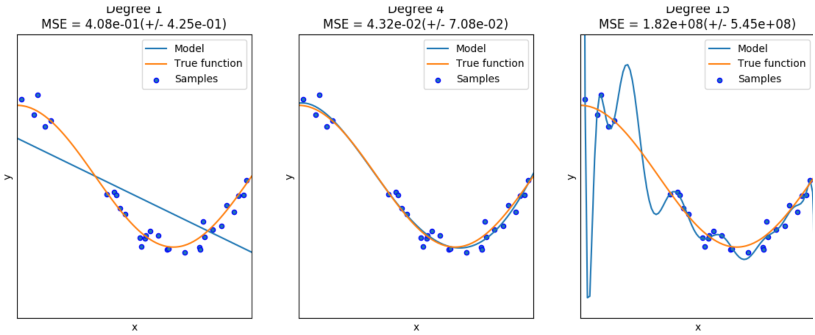
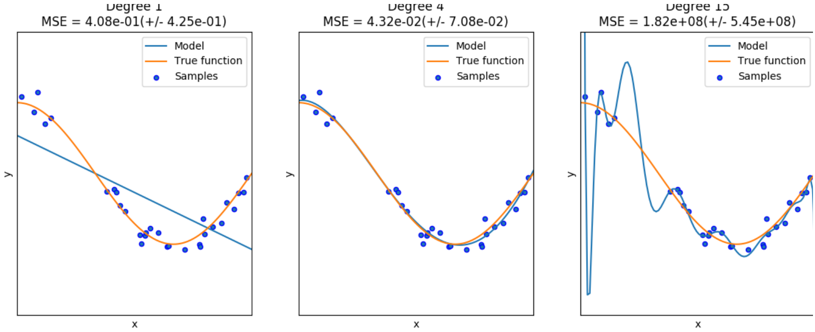


Underfitting vs. Overfitting



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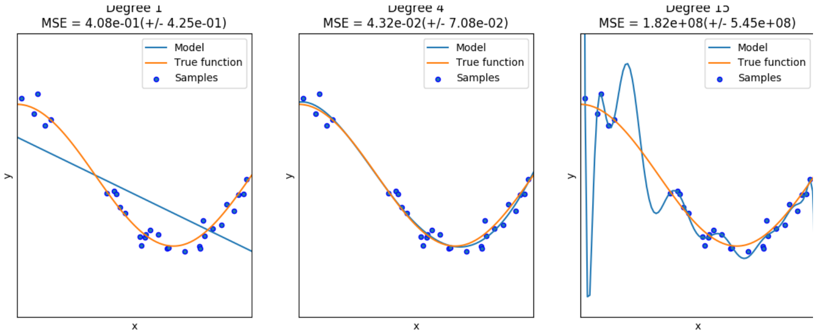

- Underfitting: Not fitting well the data (large MSE).

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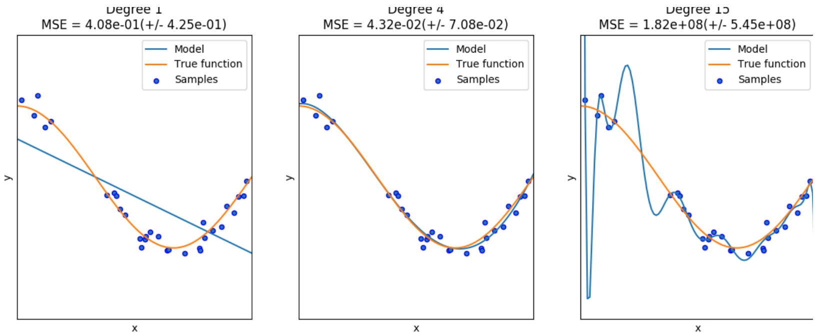

- Underfitting: Not fitting well the data (large MSE).
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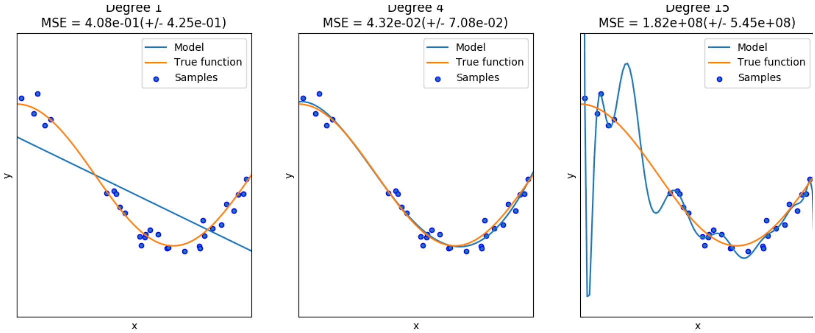

- Underfitting: Not fitting well the data (large MSE).
- Overfitting: We are “learning the noise” (small MSE).

Adding complexity can lead to overfitting and thus worse generalization.

Underfitting vs. Overfitting

Mitigation measures:

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Underfitting vs. Overfitting

Mitigation measures:

1. Estimate the model parameters on a training set
2. Large MSE $\Rightarrow$ underfitting
3. Small MSE $\Rightarrow$ Test on a validation set
4. Large MSE on the validation $\Rightarrow$ overfitting $\Rightarrow$ bad generalization

To recap, overfitting happens with small training error and large validation error

Not done yet

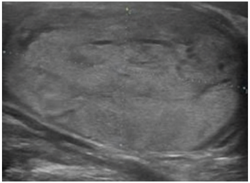
So is polynomial regression all we need?

Not really!

- Different loss than MSE
- Regularization
- Additional priors
- Intermediate features
- Regression (predict a value) vs. classification (predict a category)

Classification

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

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

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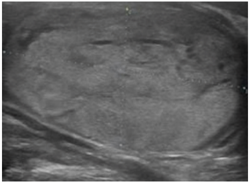
$f_{\Theta}($  $) = \{0, 1\}$

Let's see how to modify the loss to minimize over categorical values directly.

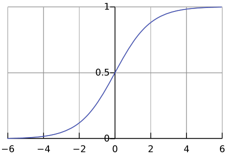
Logistic regression

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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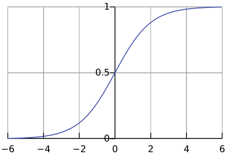

σ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

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$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} (y_i - \sigma(\underbrace{ax_i + b}_{\text{linear}}))^2 \qquad \textcolor{red}{\texttt{non-convex in } a, b}$$

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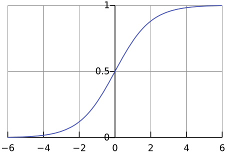

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New loss:

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

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

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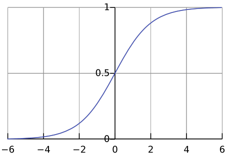

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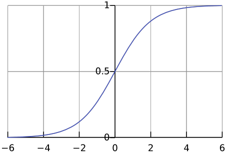

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New convex loss:

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

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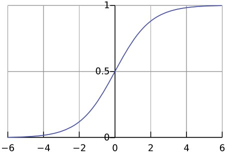

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Logistic regression: Finding a solution

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

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

Logistic regression: Finding a solution

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

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

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Consider the gradient of each term in the summation:

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

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Apply the chain rule to each partial derivative:

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

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Consider the gradient of each term in the summation:

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

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

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

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

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Apply the chain rule to each partial derivative:

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

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

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

Logistic regression: Finding a solution

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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:

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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:

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

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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