Deep Learning & Applied AI

Overfitting and going nonlinear

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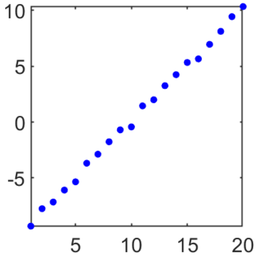
A glimpse into neural networks

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

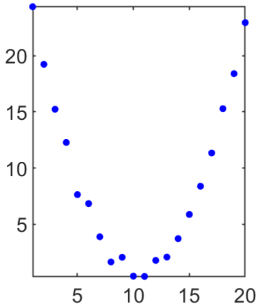
$$f_{\boldsymbol{\Theta}}(\mathbf{x}) = \mathbf{y}$$

Parametrized models

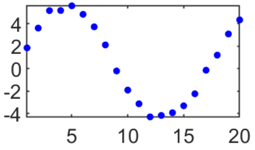
The parameters describe the behavior of the network, and must be solved for.



$$y = ax + b$$



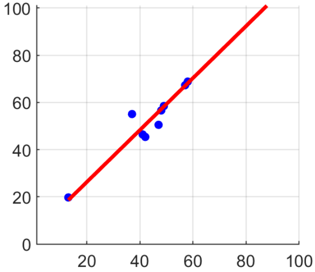
$$y = ax^2 + bx + c$$



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

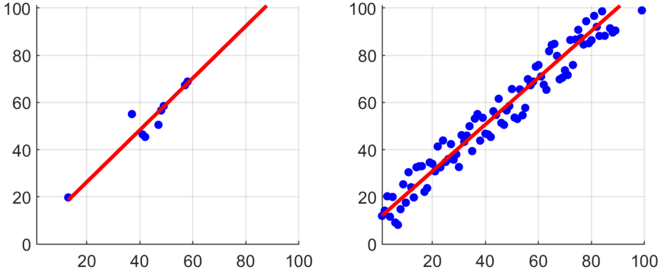
From a technical standpoint, our task is to determine the parameters Θ.

Data distribution



Assumption: linear model

Data distribution



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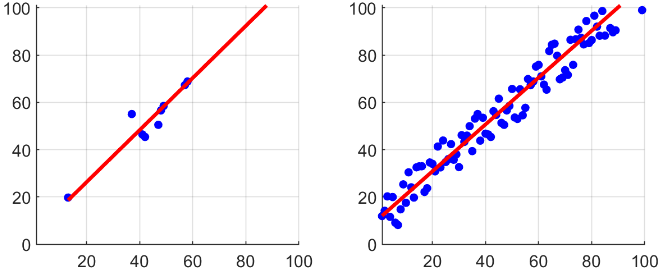
More data allows us to improve our prediction

Data distribution

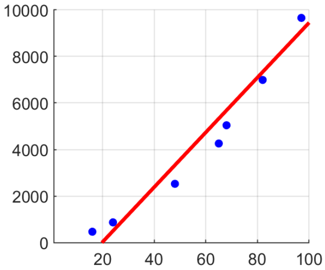


Assumption: linear model

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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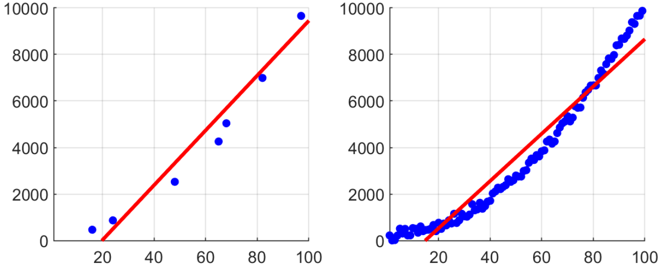
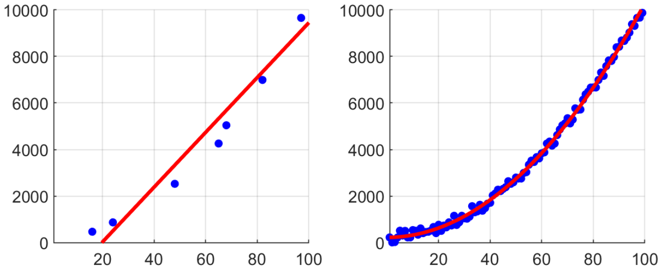


Assumption: linear model

More data confutes our assumptions

Data distribution



Assumption: quadratic model

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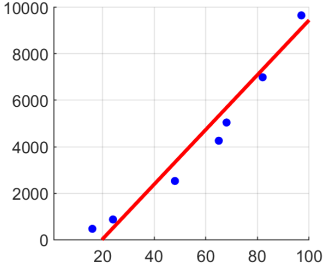

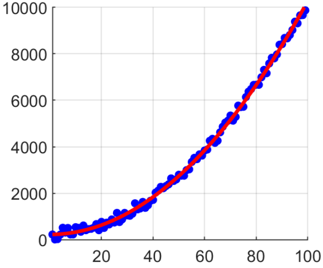

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Key questions:

- How to select the correct distribution?

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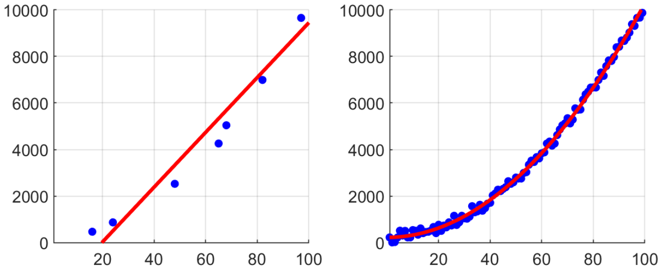

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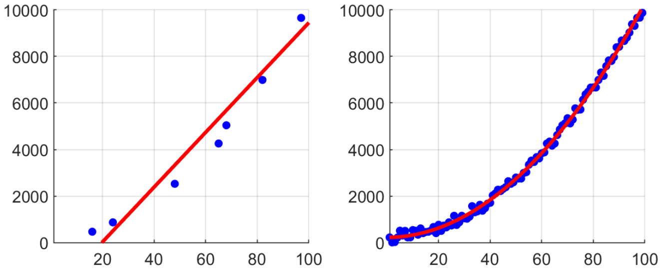


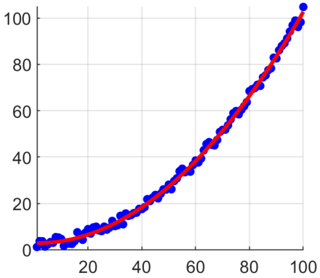
Assumption: quadratic model

Key questions:

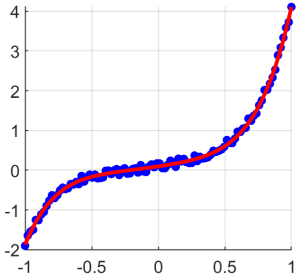
- How to select the correct distribution?
- How much data do we need?
- What if the correct distribution does not admit a simple expression?

Polynomial regression

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



2nd-order



5th-order

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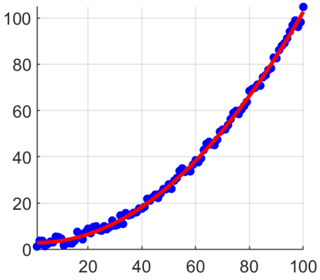

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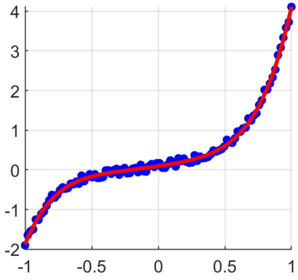

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The number of parameters grows with the order.

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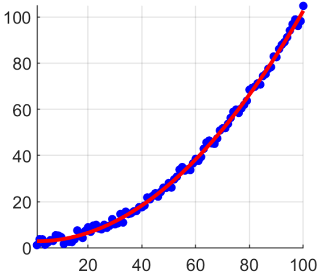

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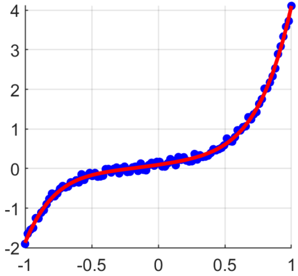

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The number of parameters grows with the order.

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

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Remark: Despite the name, polynomial regression is still linear in the parameters. It is polynomial with respect to the data.

Linear regression with polynomial features

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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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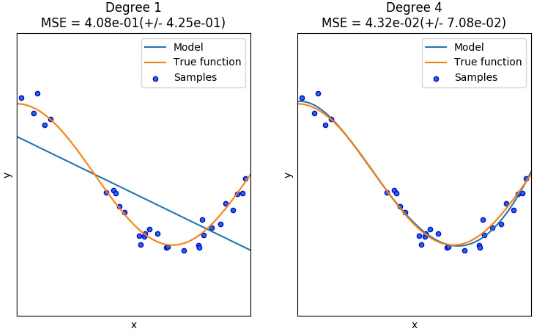

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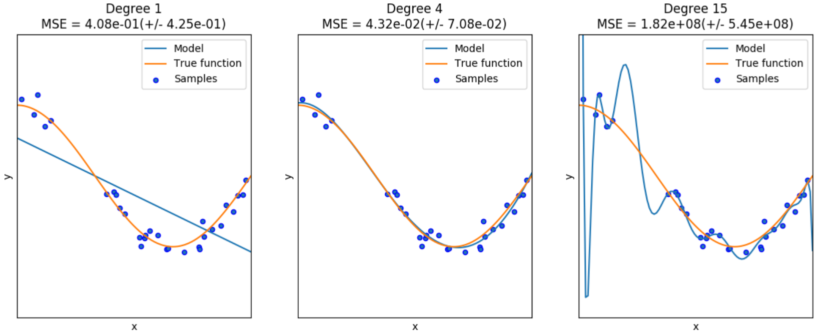
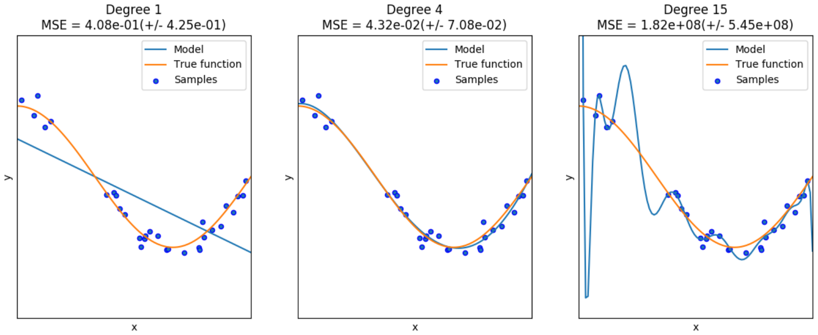


Underfitting vs. Overfitting



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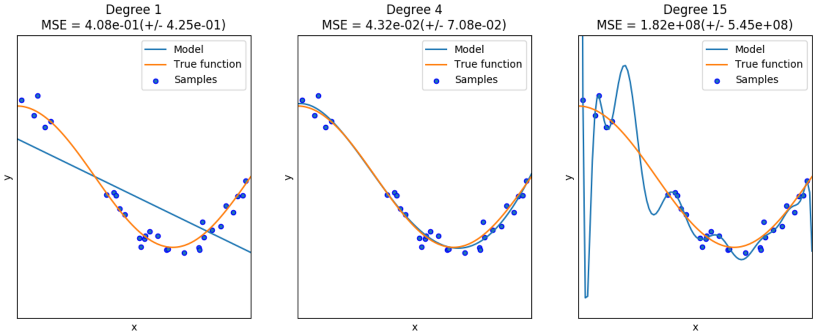

- Underfitting: Not sufficiently fitting the data (large MSE).

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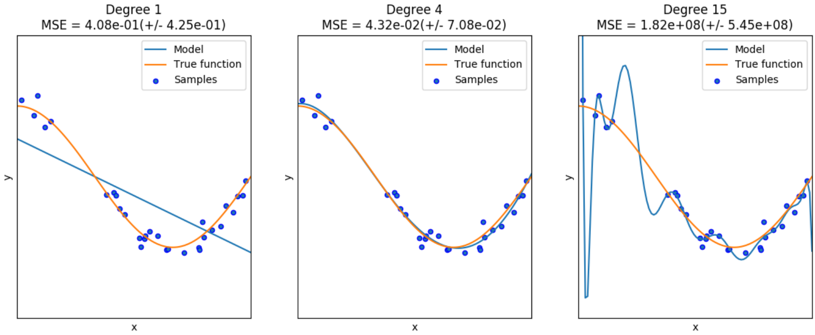

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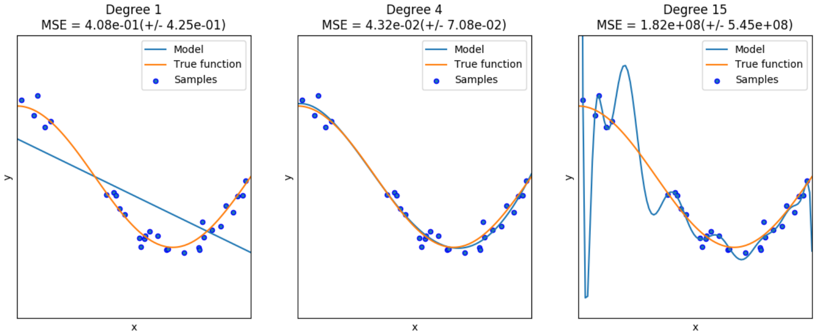

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Adding complexity can lead to overfitting and thus worse generalization.

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Different mechanisms defend us from under- and overfitting.

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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

"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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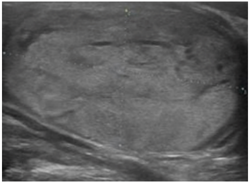
So is polynomial regression all we need?

Not really!

- Different loss than MSE
- Regularization
- Additional priors
- Intermediate features
- Flexibility
- 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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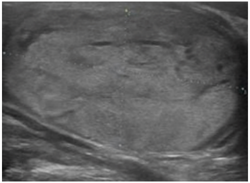
$f_{\Theta}($  $) = \{0, 1\}$

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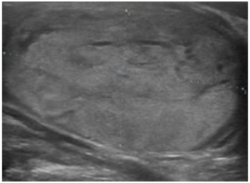
$f_\Theta($  $) = \{0, 1\}$

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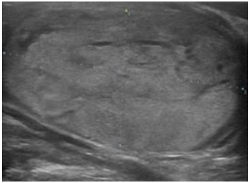
$f_\Theta($  $) = \{0, 1\}$

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.

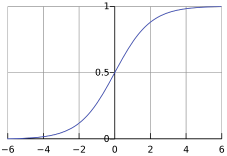
Logistic regression

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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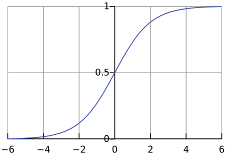

σ has a saturation effect as it maps $\mathbb{R} \mapsto (0, 1)$.

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

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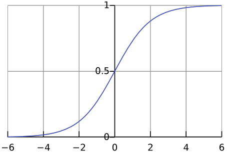

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$$\ell_\Theta(\{x_i, y_i\}) = \sum_{i=1}^{n} c(x_i, y_i)\,, \quad \text{with}$$

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

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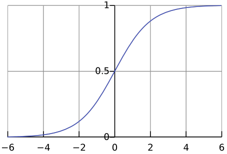

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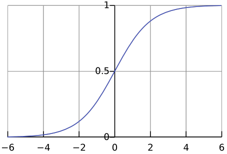

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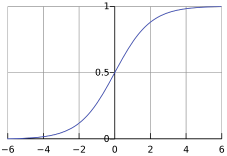

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Logistic regression: Finding a solution

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

$$\nabla_\Theta \ell_\Theta = 0$$

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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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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:

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

Apply the chain rule to each partial derivative:

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

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

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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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By looking at the partial derivative:

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

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linear regression	convex	
linear regression + Tikhonov	convex	
logistic regression	convex	

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

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linear regression	convex	least squares
linear regression + Tikhonov	convex	least squares
logistic regression	convex	

Logistic regression: Finding a solution

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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