Linear regression and Optimisation

Introduction to Machine Learning - Tutorial 2

Piersilvio De Bartolomeis

Simplified diagram of supervised learning

Training Data

(x_1, y_1)
$\vdots$
(x_n, y_n)

attributes of patient

supervision: observed labels

ML method: efficiently find $\hat{f} \in \mathscr{F}$ that fits training data

ML scientists design

Some test input x

Model $\hat{f}$

Prediction $\hat{f}(x)$

Recap from last week: Linear regression

Training Data

ML method:
efficiently find $\hat{f} \in \mathcal{F}$

Model $\hat{f}$

ML Scientists
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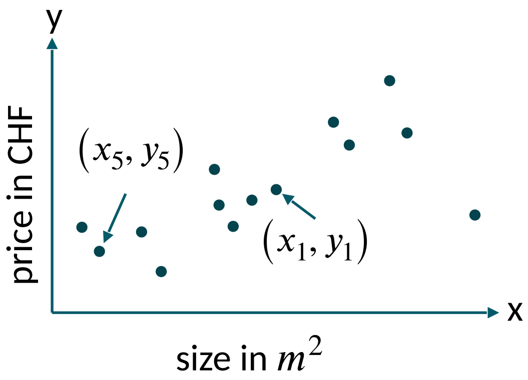
Function class	Training loss	Optimisation
• linear functions	• squared loss	• closed-form

Recap from last week: Linear regression

Training Data

$$\begin{matrix}(x_1, y_1)\\ \vdots \\ (x_n, y_n)\end{matrix}$$



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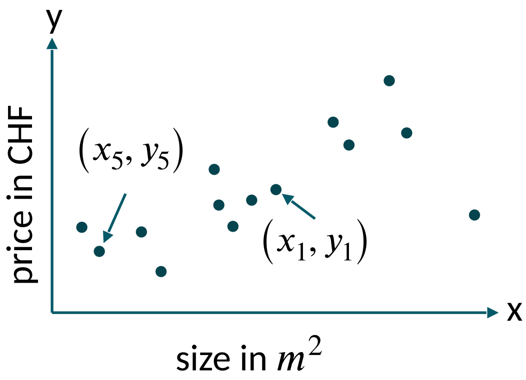
$$w^* = \operatorname{argmin}_{w \in \mathbb{R}^2} \frac{1}{2n} \|y - \Phi w\|^2$$



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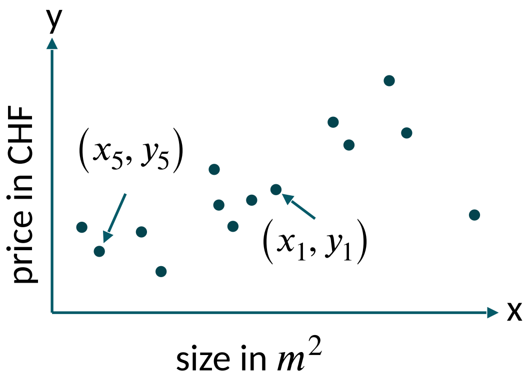
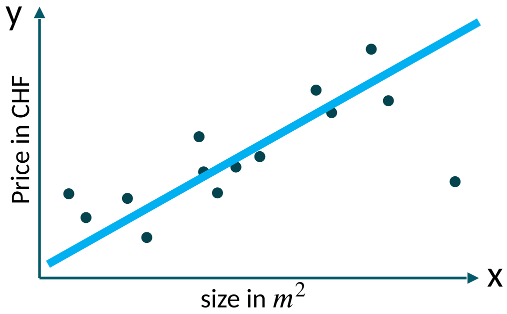
Model $\hat{f}$

$$\hat{f}(x) = x^\top w^*$$





Intermezzo: Convex functions

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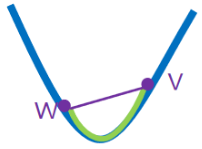

Mathematically, convexity is the function property that guarantees local = global minimum

- 0-th order condition (if and only if): $L(\lambda w + (1-\lambda)v) \leq \lambda\, L(w) + (1-\lambda)L(v)$

  true function connecting any w, v $\leq$ linear function connecting two points x, y

Intermezzo: Convex functions

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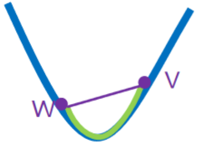

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- 1st order condition (if and only if): $L(v) \geq L(w) + \nabla L(w)^{\top}(v-w)$

  value at any v of tangent line at any w $\leq$ true value at v

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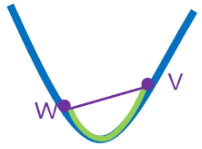

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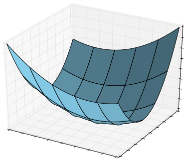

- 2nd order condition (if and only if): Hessian $\nabla^2 L(w) \succcurlyeq 0$

  non-negative curvature at every $\mathbf{w}$

Recap from last week: Closed-form solution

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(i) Define opt. problem: $w^* = \operatorname*{argmin}_{w \in \mathbb{R}^d} \overbrace{\frac{1}{2n} \|y - \Phi w\|^2}^{=L(w)}$

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This week so far

Training Data

ML method:
efficiently find $f \in \mathscr{F}$

Model $\hat{f}$

ML Scientists
design

Function class

Training loss

Optimisation

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Training Data → ML method: efficiently find $f \in \mathcal{F}$ → Model $\hat{f}$

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Function class	Training loss	Optimisation
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Function class	Training loss	Optimisation
• linear	• squared loss	• gradient descent
• polynomial	• mae loss	• momentum
• trigonometric	• huber loss	• adaptive methods

Today!

Recap from this week: Polynomial regression

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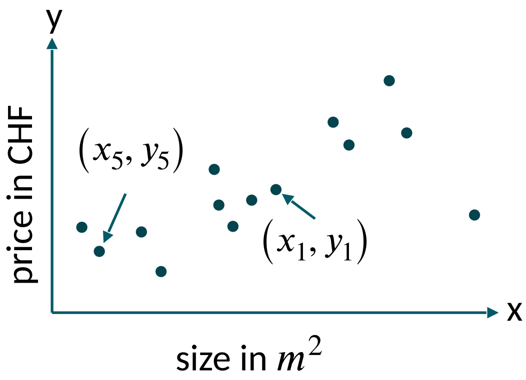

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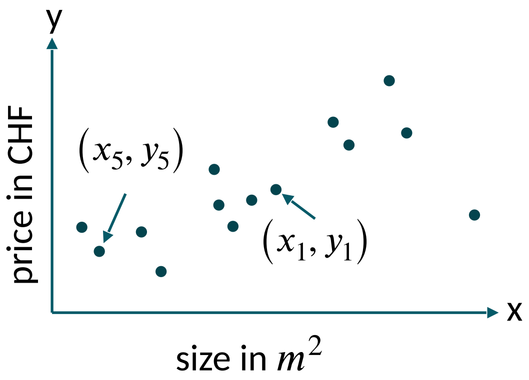

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$$\begin{matrix}(x_1, y_1)\\ \vdots \\ (x_n, y_n)\end{matrix}$$

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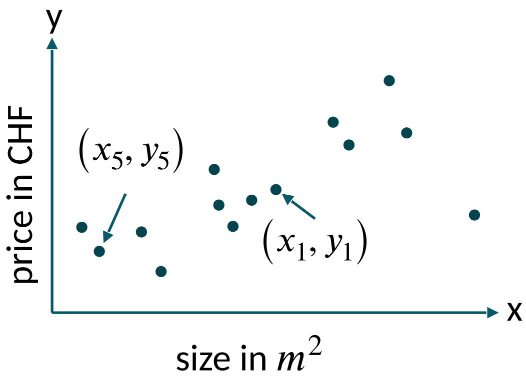
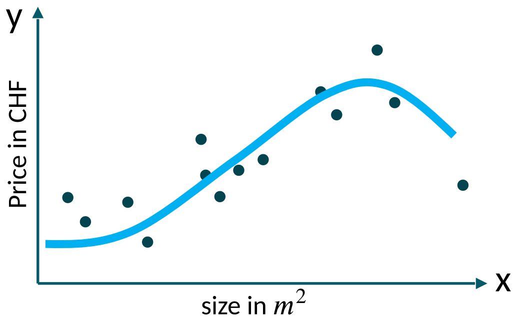
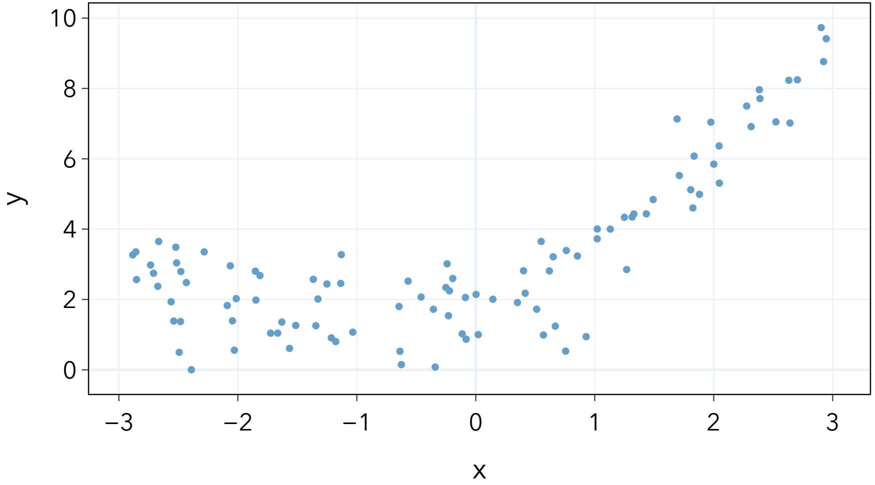




Recap from this week: Polynomial regression

What to do if we want to fit $\hat{f}(x) = w_0 + w_1 x + w_2 x^2$?



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(iii) The design matrix becomes $\Phi = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}$

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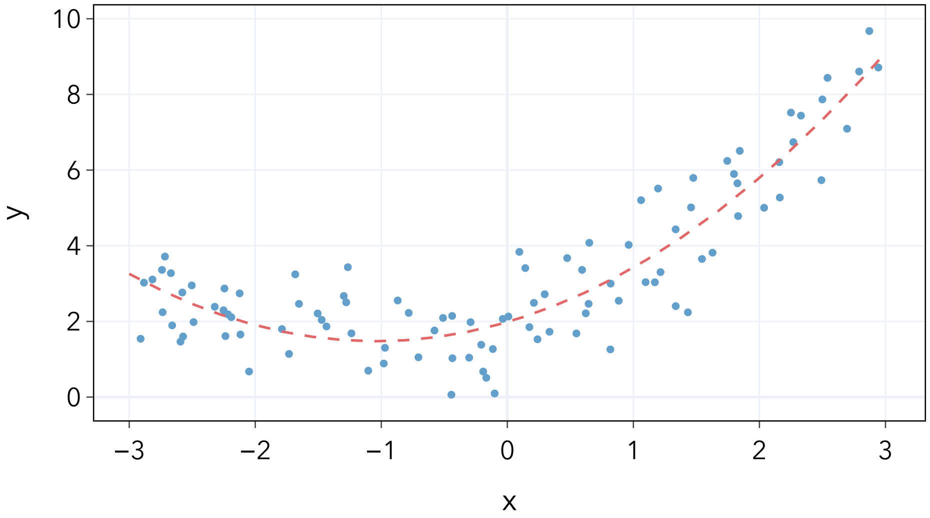
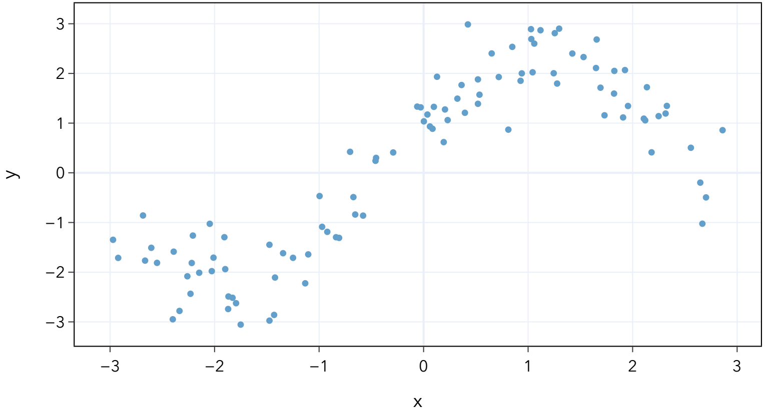
Recap from this week: Polynomial regression

How does our fit look like? $\hat{f}(x) = \phi(x)^\top w*$



Beyond polynomials: Trigonometric functions

What to do if we want to fit $\hat{f}(x) = w_1 \sin(x) + w_2 \cos(x)$?



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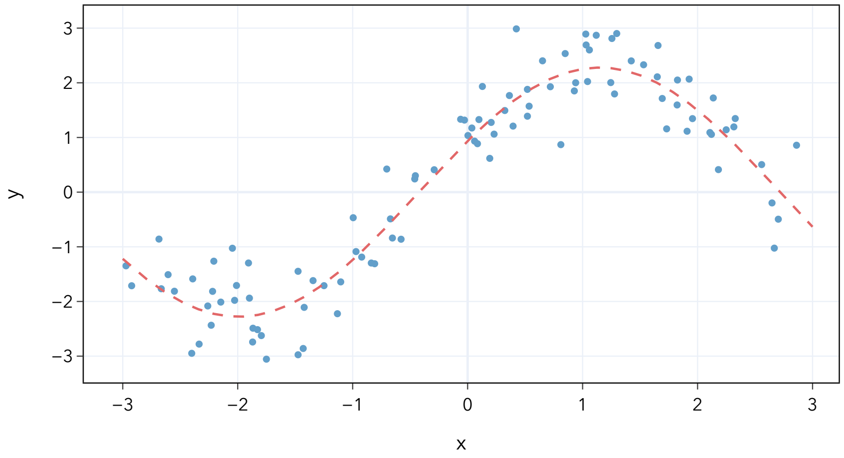

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More on Jupyter!

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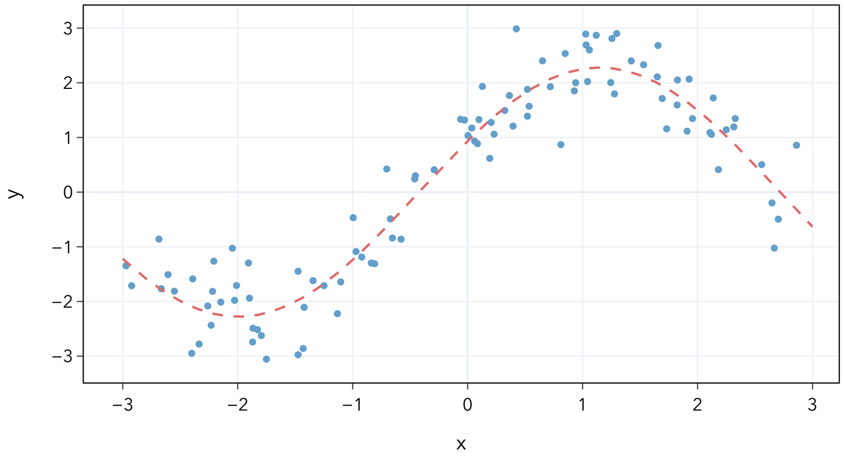


Recap from this week: Gradient descent algorithm

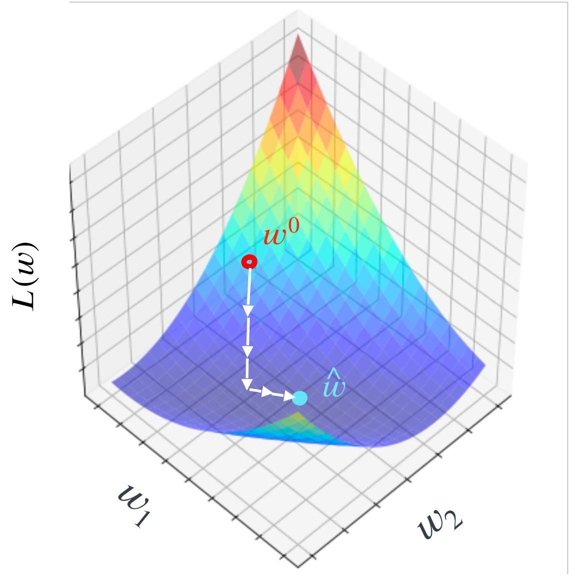
Gradient descent algorithm to minimize $L(w)$

Start at initial w^0

At each step t, $w^{t+1} = w^t + \eta \nabla_w L\left(w^t\right)$

Stop e.g. when $|L(w^{t+1}) - L(w^t)| \leq \epsilon$

Output $\hat{w} = w^{final}$



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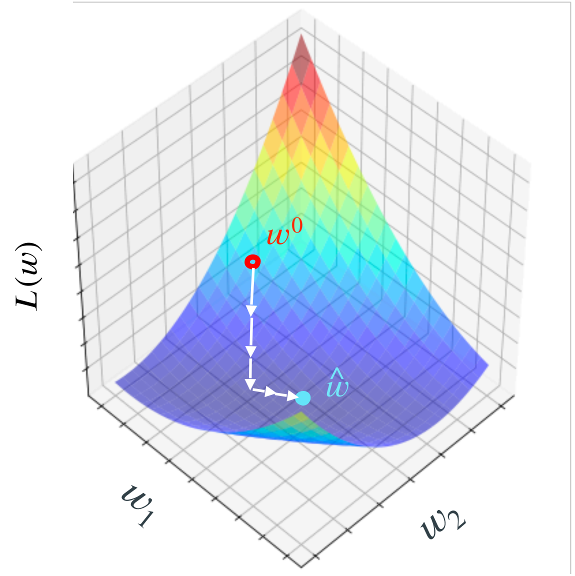

Linear approximation for the loss value at step $t+1$

$$L\left(w^{t+1}\right) = L\left(w^t - \eta \nabla L(w^t)\right) \approx L\left(w^t\right) - \eta \left\langle \nabla L\left(w^t\right), \nabla L\left(w^t\right) \right\rangle < L(w^t)$$

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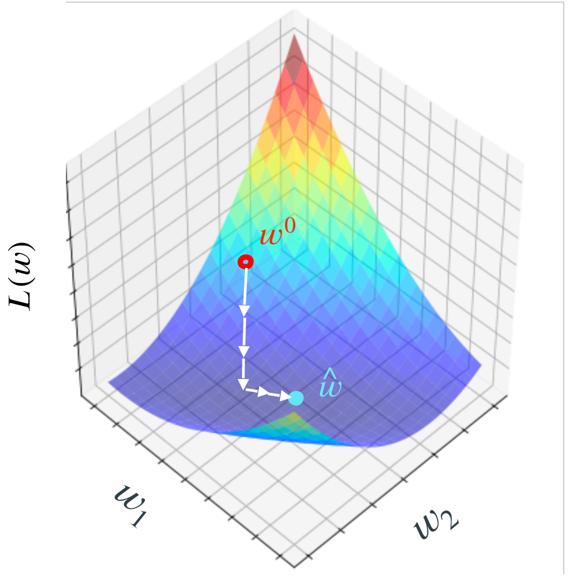

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the negative gradient direction is a descent direction

for small enough stepsize η

Gradient descent: how fast does it converge?

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- Question: when does gradient descent converge and how fast?

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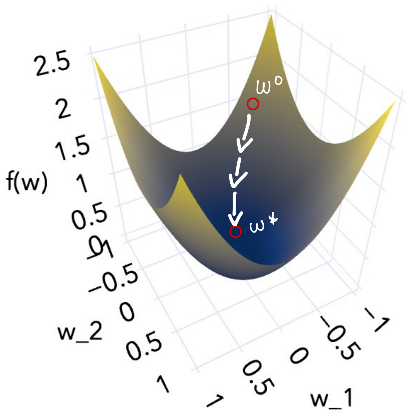

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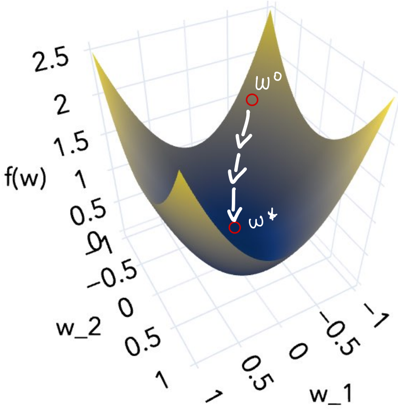
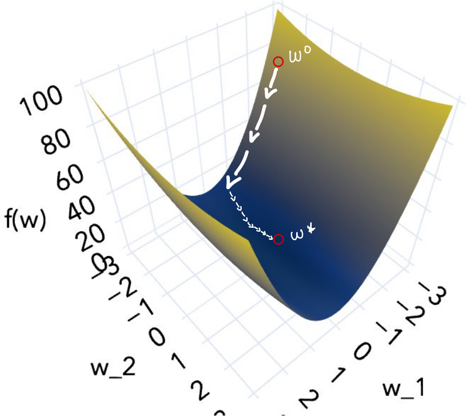


$A = \begin{pmatrix} 1 & 0 \\ 0 & 5 \end{pmatrix}$



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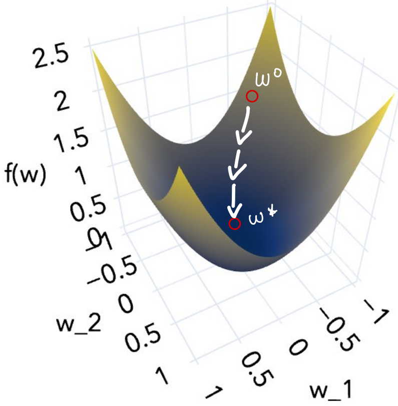

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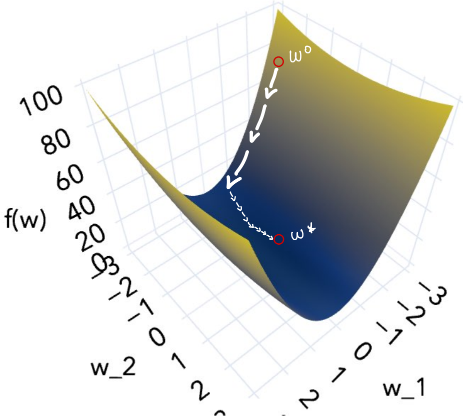

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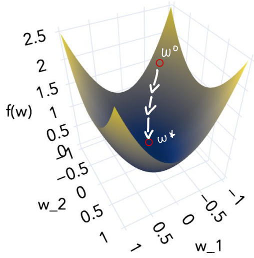
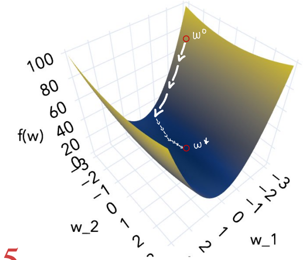


$\kappa = 1$



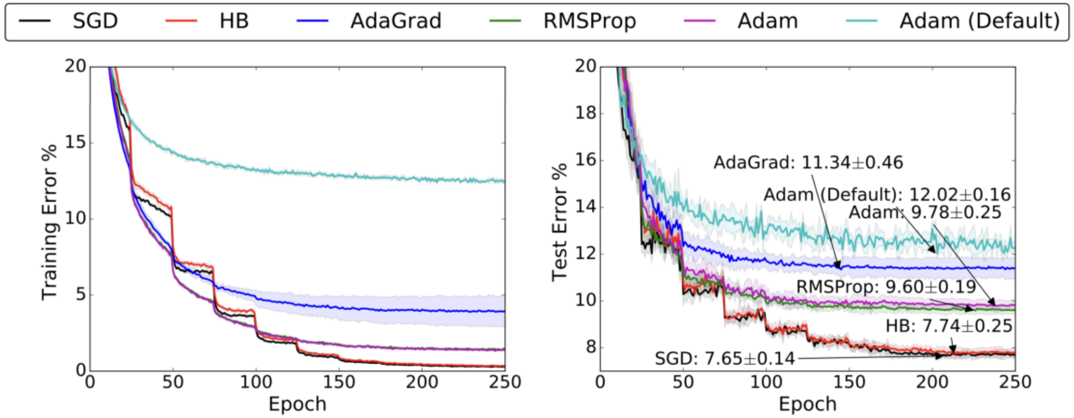
$\kappa = 5$

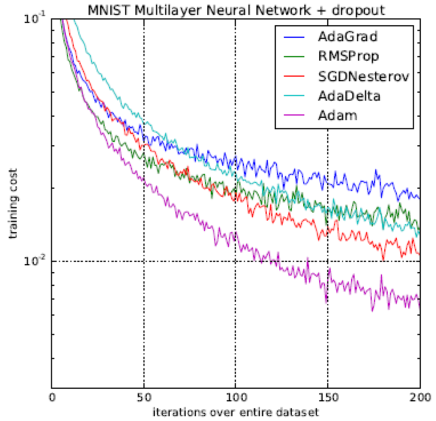
There’s a whole zoo of optimisation methods…

For deep learning, there are many optimisation methods (number of lines)

people usually try out (don’t have to understand plots in detail)

→ now want to have a brief overview how they differ from gradient descent





Speeding up gradient descent

Goal: Large steps in flat areas, small steps in high curvature ones, dampened oscillations

- momentum/accelerated methods: combine previous direction with neg. gradient direction for some $\alpha \in \mathbb{R}$

$$w^{t+1} - w^t = \alpha \left(w^t - w^{t-1}\right) - \eta \nabla_w L\left(w^t\right)$$

(bonus: discrete approximation of dampened harmonic oscillator)

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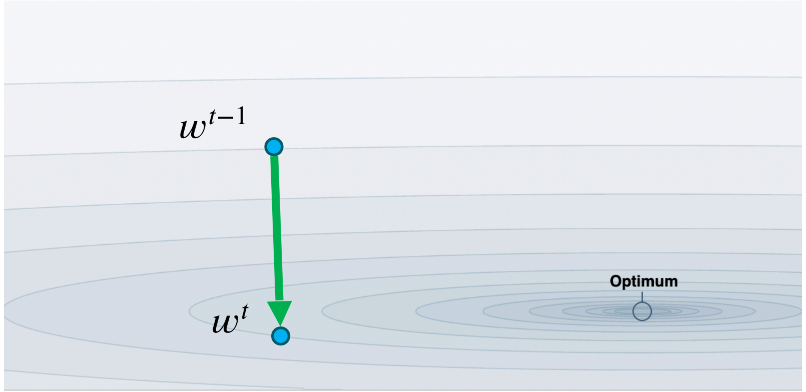
how it dampens oscillations



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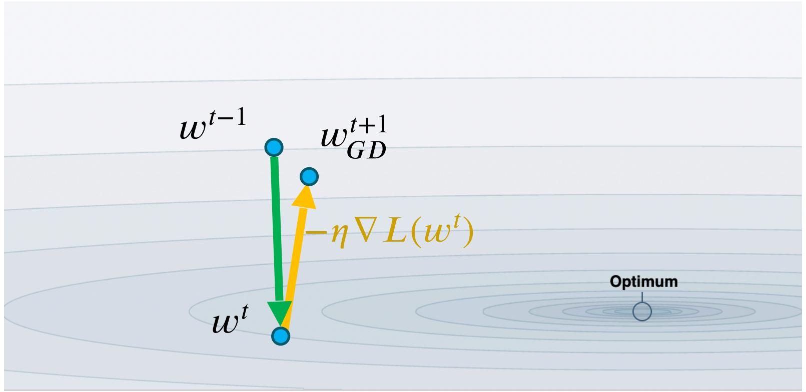
$$w^{t+1} - w^t = \alpha\left(w^t - w^{t-1}\right) - \eta \nabla_w L\left(w^t\right)$$

(bonus: discrete approximation of dampened harmonic oscillator)

At time step t:

neg. gradient direction at step t

how it dampens oscillations



Speeding up gradient descent

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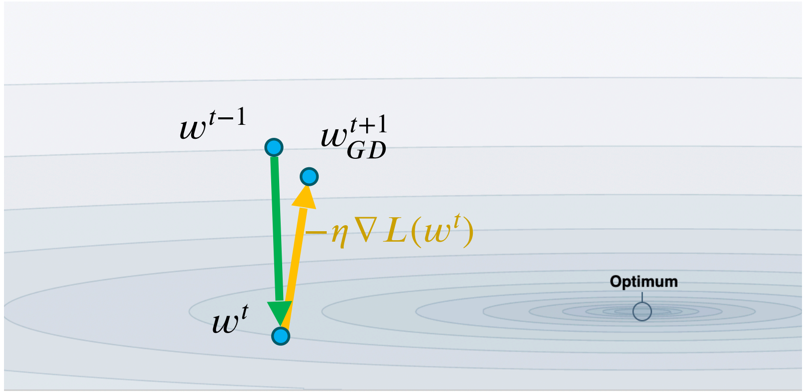

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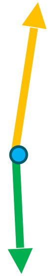

(scaled) direction in step $t-1$: $w^t - w^{t-1}$

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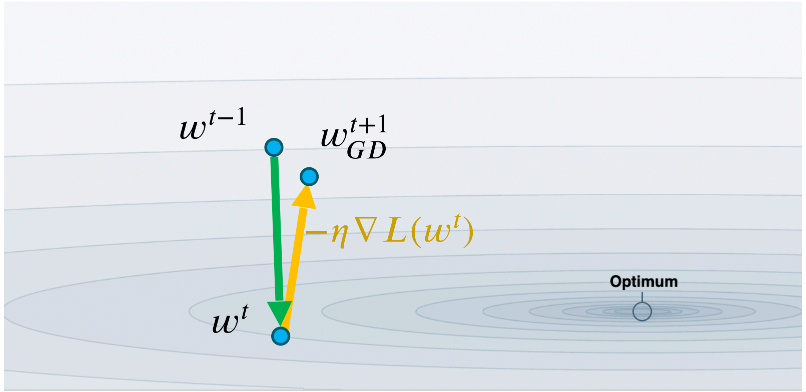

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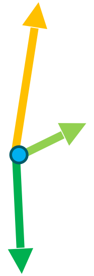

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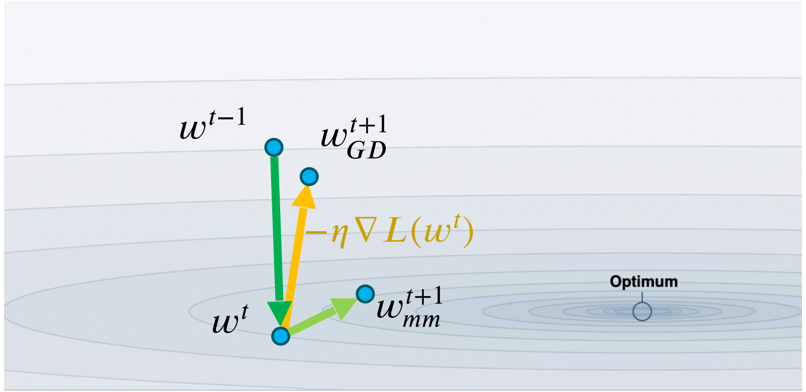

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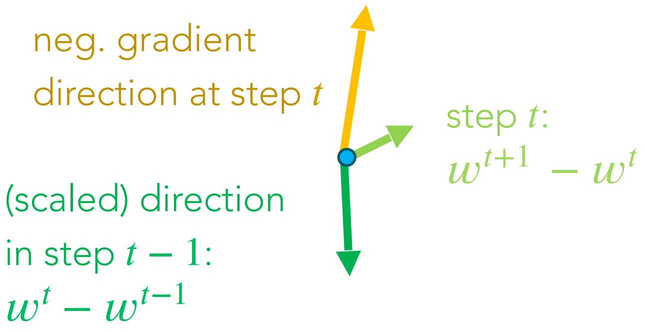

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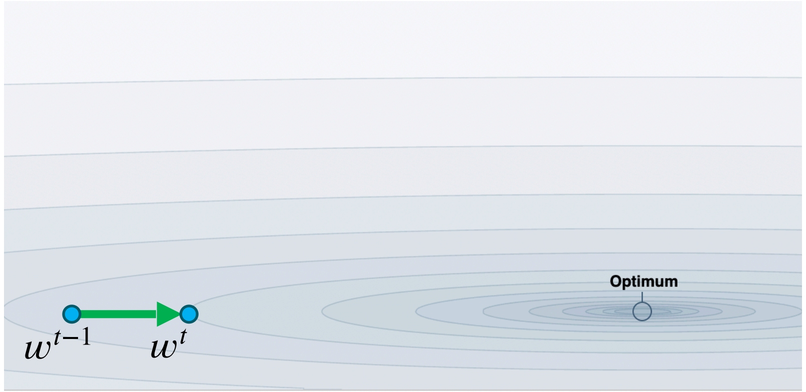

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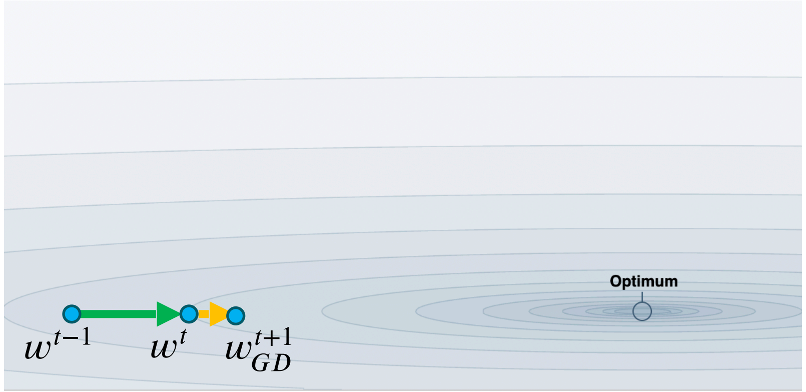

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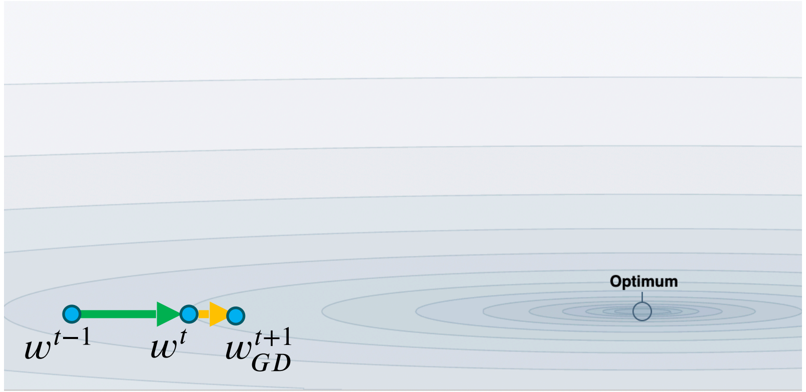

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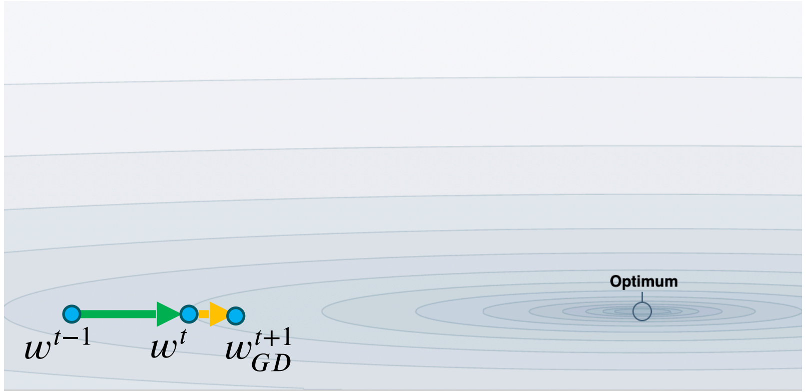

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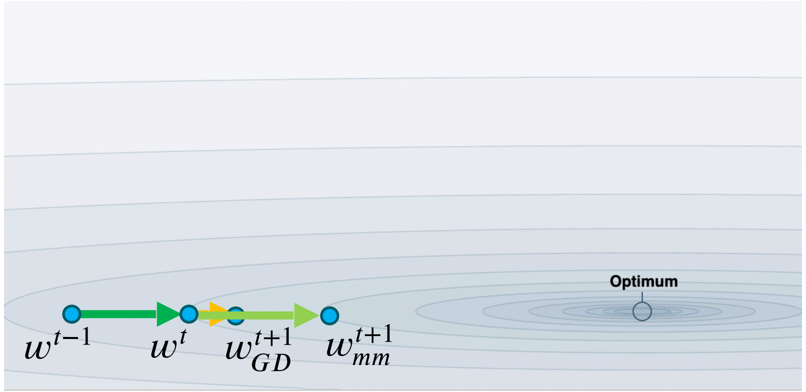

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  intuitively: the elements i which already changed a lot, have smaller stepsize

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Nice overview blog posts: https://distill.pub/2017/momentum/; https://ruder.io/optimizing-gradient-descent/index.html

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More on Jupyter!

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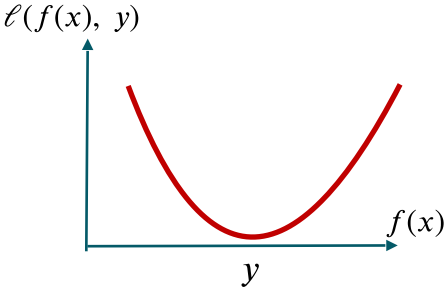

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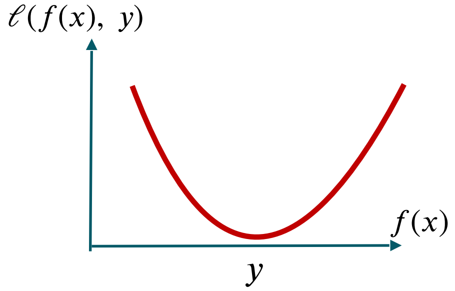

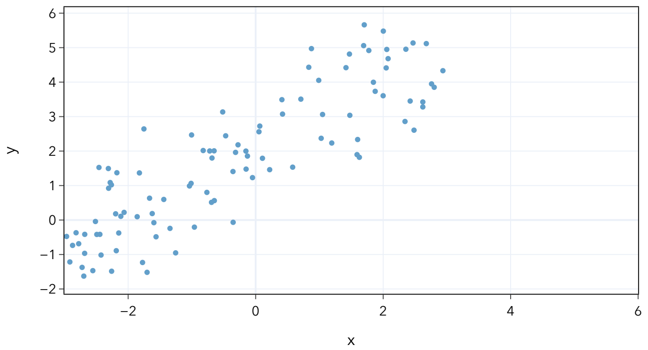

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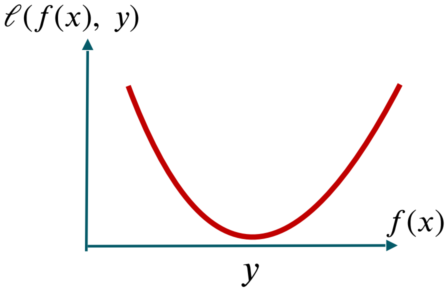

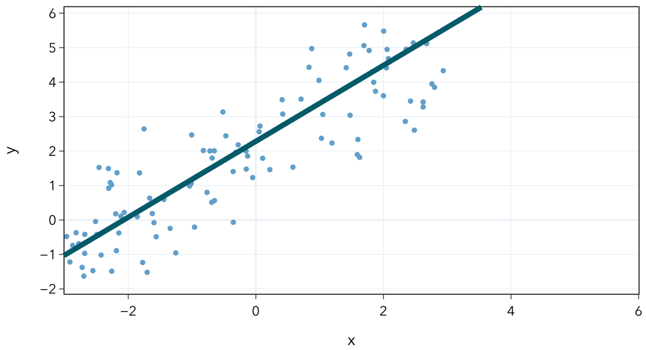

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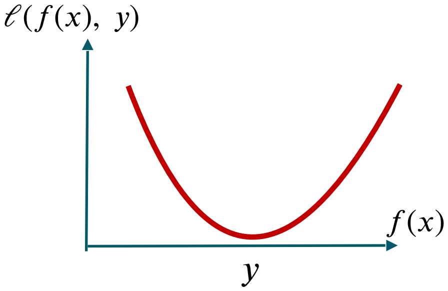

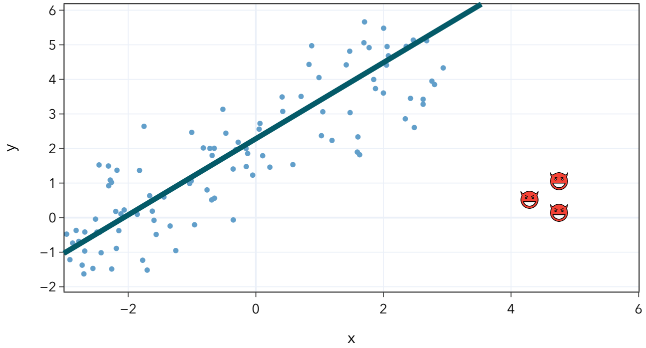

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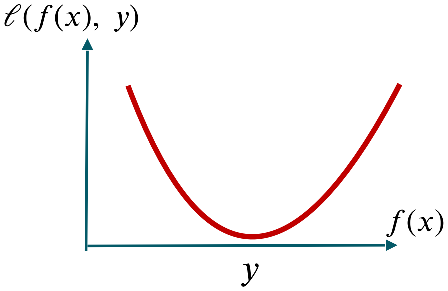

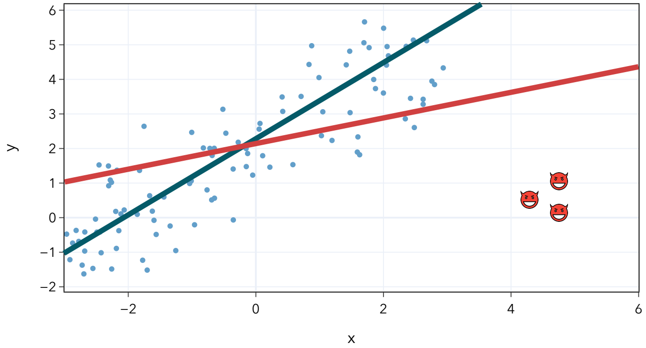

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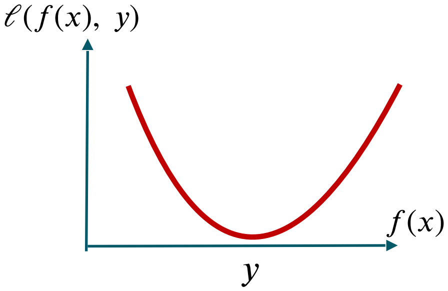

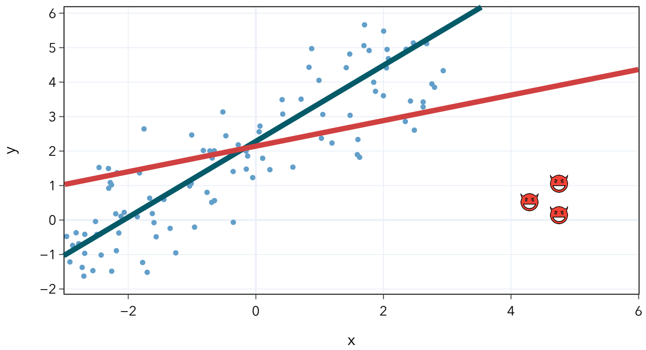

Grows quadratically: huge penalty for large errors!

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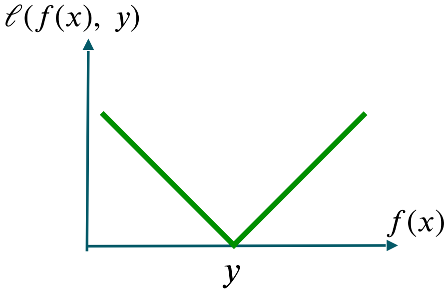

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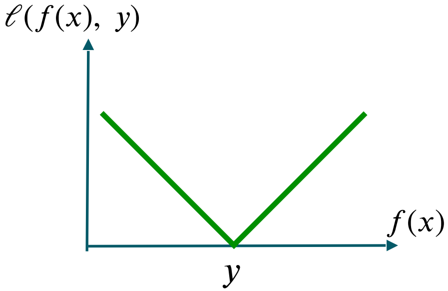

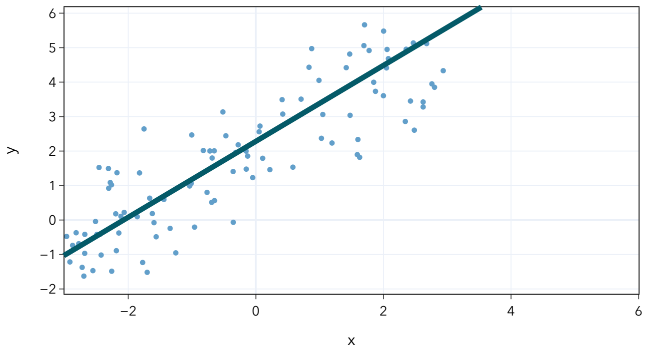

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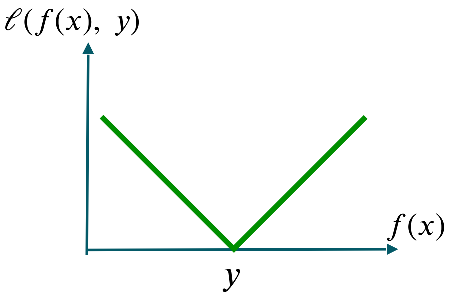

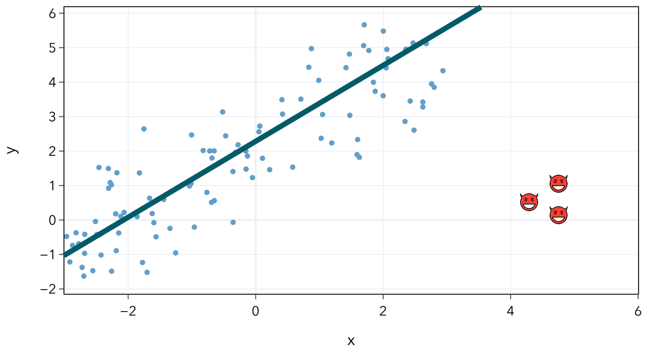

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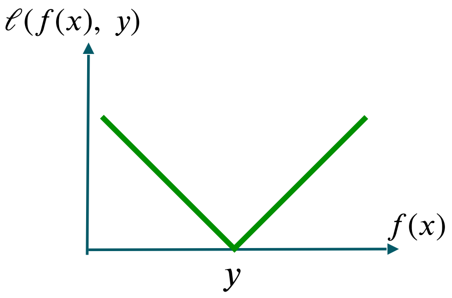

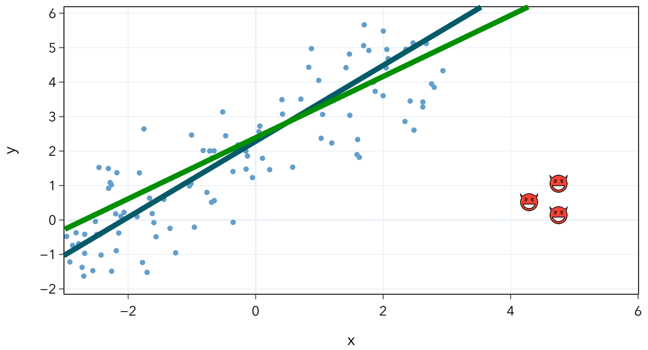

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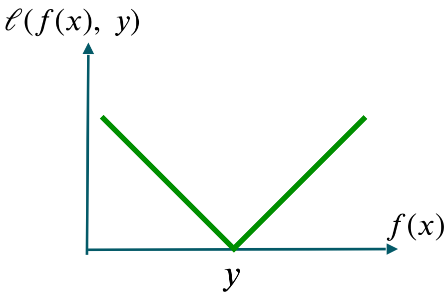
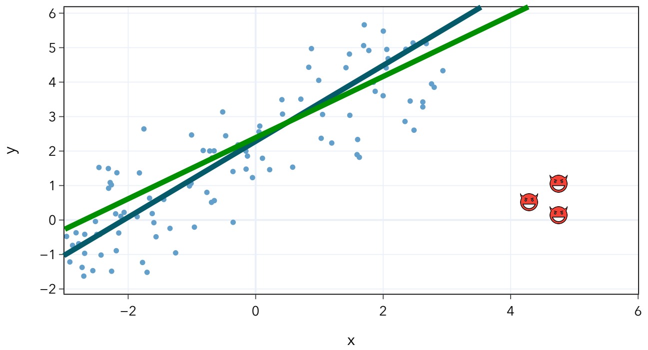
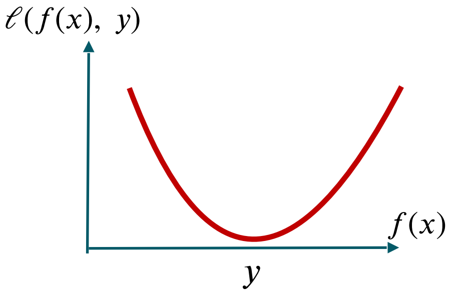




Grows linearly: smaller penalty for large errors!

Mean absolute error is not differentiable

$\ell_{\text{square}}(f(x), y) := (y - f(x))^2$



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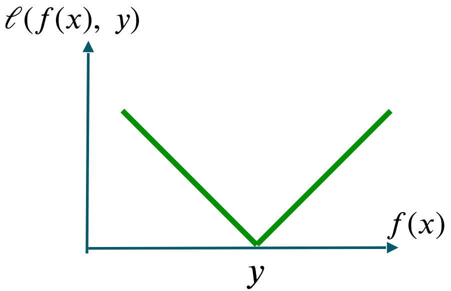

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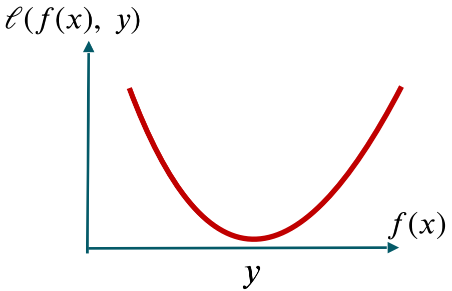

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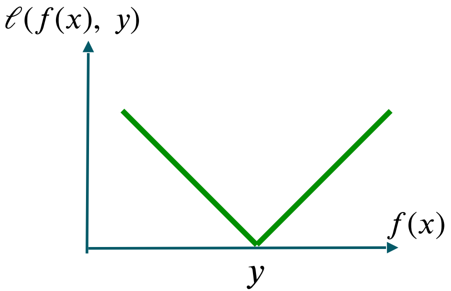

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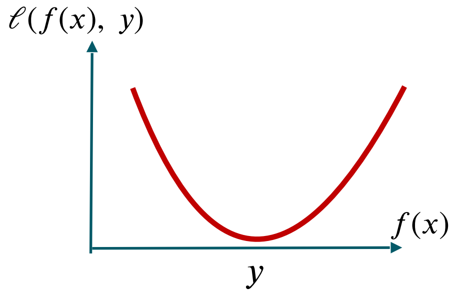

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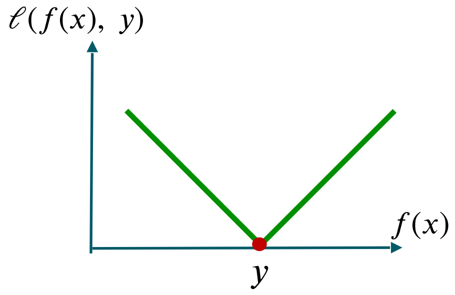

Not differentiable at $f(x) = y$

Best of both worlds: Huber loss

Can we combine ℓ_{square} and ℓ_{abs} in a differentiable function?

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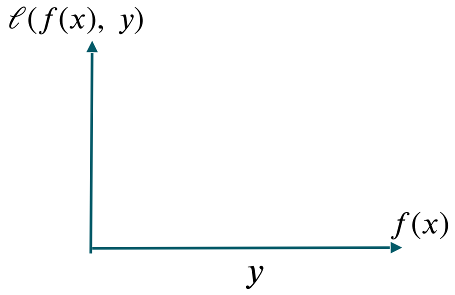

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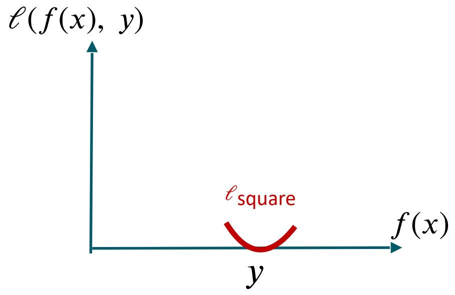

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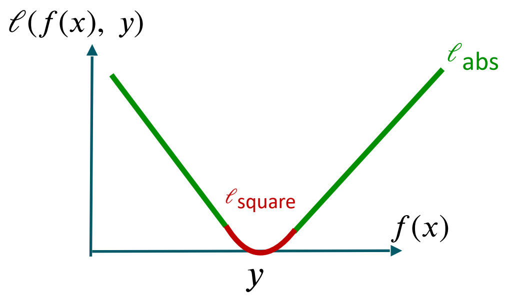

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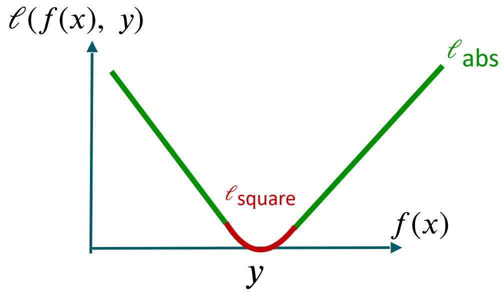

$$\ell_{\text{huber}}(f(x), y) := \begin{cases} (y - f(x))^2 & \text{if } |y - f(x)| \leq \delta \\ 2\delta|y - f(x)| - \delta^2 & \text{else} \end{cases}$$

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More on iPad and Jupyter!

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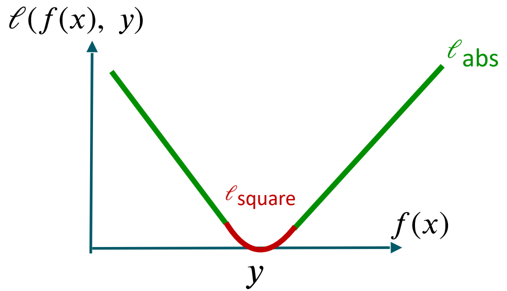

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