Machine Learning: Optimization 1

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- For mean-squared error

$$L = \sum_{i=1}^{n} (w^\top x_i - y_i)^2 = \|Xw - y\|_2^2, \tag{1}$$

we know that

$$w^* = (X^\top X)^{-1} X^\top y \tag{2}$$

is the solution of $\nabla_w L = 0$.

- How do we know w^* is the optimal point?

- For log loss

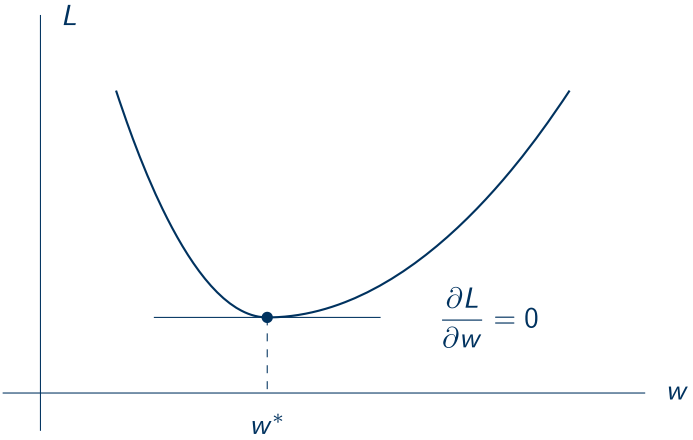
$$L = \sum_{i=1}^{n} \log\left(1 + \exp(-y_i w^\top \phi(x_i))\right) \tag{3}$$

we cannot even solve $\nabla_w L = 0$.

- How do we find the optimal solution?

- Could we find an approximate solution?

Convex optimization



Optimization

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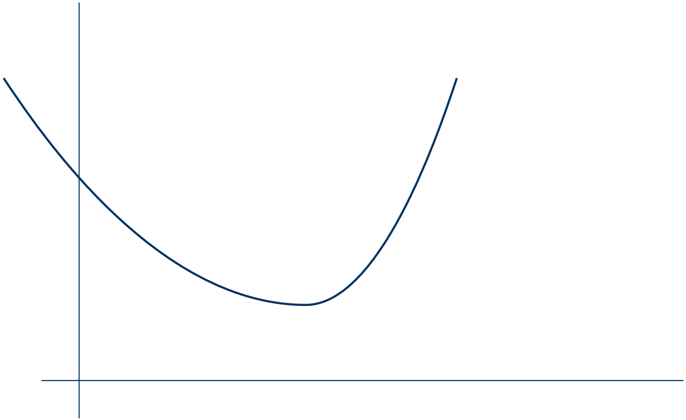
- The point x^* is called the **optimal solution** or the **minimizer** of f.
- There might not be a minimizer or there might have many, not just one. (In most case, we are content with finding one.)

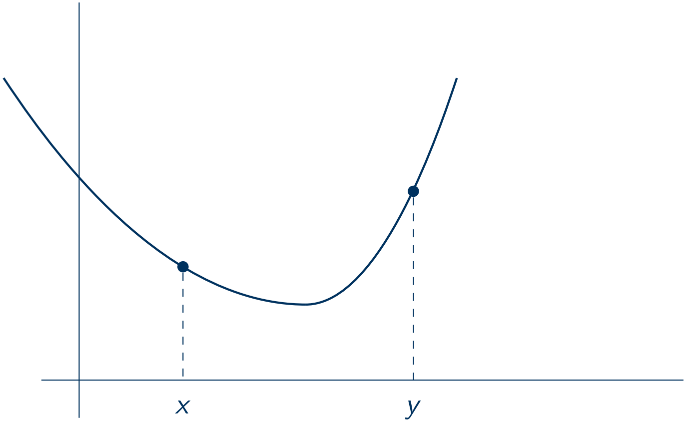
Convex functions

A function f is **convex** if

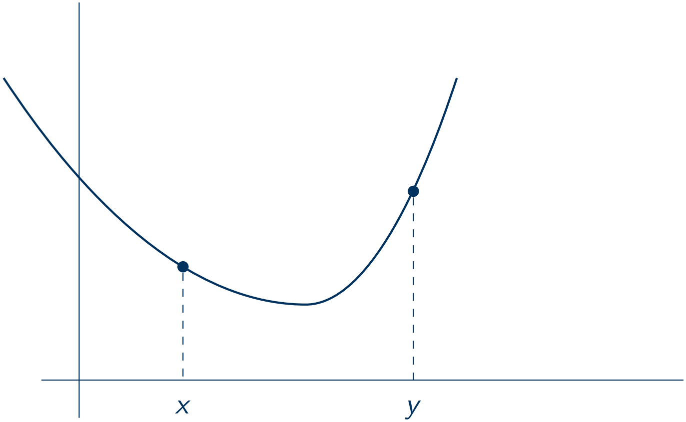
$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y), \tag{5}$$

for every x, y, and $0 \leq \alpha \leq 1$.

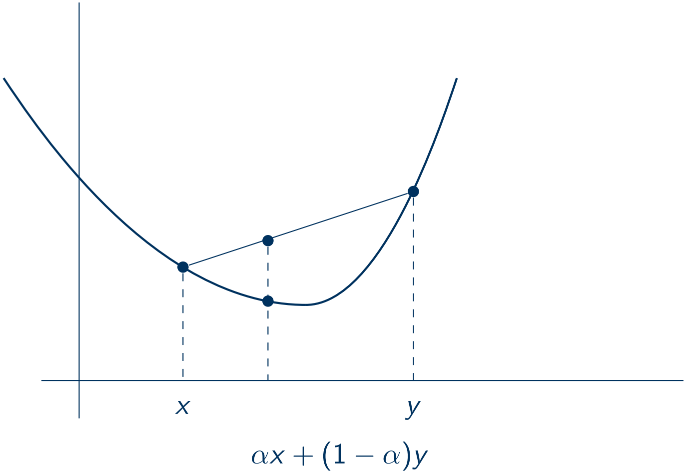




x
y



$\alpha x + (1-\alpha) y$


x
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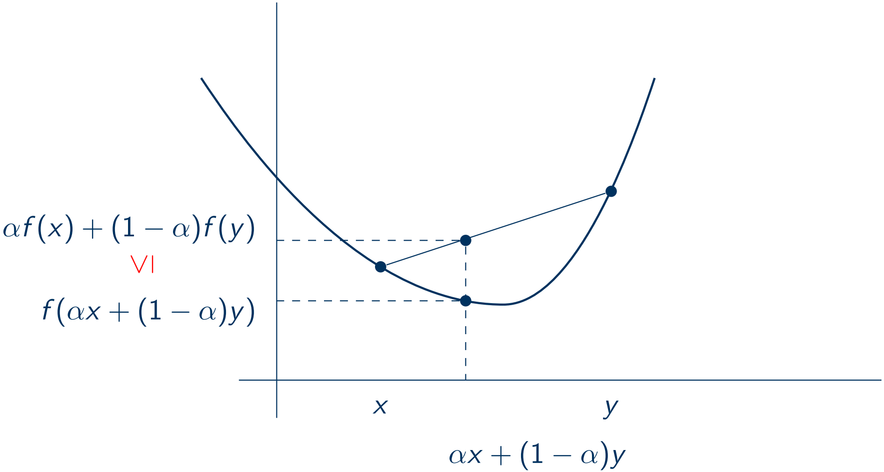
$\alpha f(x) + (1-\alpha) f(y)$
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Properties of convex functions

If f is convex, then

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y), \tag{6}$$

for any x and y.

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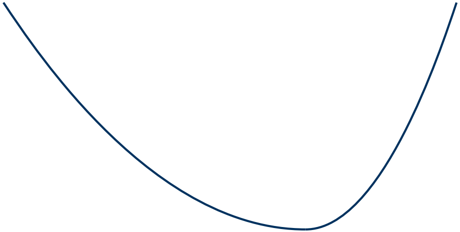
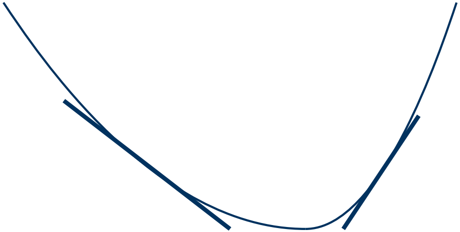
Proof:

$$\begin{aligned} f(\alpha x + (1-\alpha)y) &\leq \alpha f(x) + (1-\alpha) f(y) \\ \alpha f(y) + f(y + \alpha(x-y)) - f(y) &\leq \alpha f(x) \\ f(y) + \frac{f(y + \alpha(x-y)) - f(y)}{\alpha} &\leq f(x) \\ f(y) + \nabla f(y)^\top (x-y) &\leq f(x) \end{aligned}$$

Supporting hyperplanes



Supporting hyperplanes



- Is the mean-squared error

$$L = \|Xw - y\|_2^2 \tag{7}$$

convex in w?

- The definition itself is not always easy to use for checking convexity.

A sufficient condition: Second derivative

- A matrix H is positive semidefinite if $v^\top H v \geq 0$ for any v.
- If the Hessian of f exists and is positive semidefinite everywhere, then f is convex.

Convexity of squared distance

- The squared distance $\ell(s) = (s - s')^2$ is convex in s.

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$$\frac{\partial^2 \ell}{\partial s^2} = 2 \geq 0 \tag{8}$$

Convexity of the ℓ_2 norm

- Show that $f(x) = \|x\|_2^2$ is convex in x.

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$$\frac{\partial^2 \ell}{\partial x_i \partial x_j} = 0 \qquad \frac{\partial^2 \ell}{\partial x_i^2} = 2 \tag{9}$$

Affine transform preserves convexity

- If f is convex, then $g(x) = f(Ax + b)$ is also convex.

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$$\begin{aligned} g(\alpha x + (1-\alpha)y) &= f(\alpha(Ax+b) + (1-\alpha)(Ay+b)) && (10) \\ &\leq \alpha f(Ax+b) + (1-\alpha) f(Ay+b) = \alpha g(x) + (1-\alpha) g(y) && (11) \end{aligned}$$

Nonnegative weighted sum of convex functions

- If $f_1, \ldots, f_k$ are convex, then $f = \beta_1 f_1 + \cdots + \beta_k f_k$ is also convex when $\beta_1, \ldots, \beta_k \geq 0$

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$$
\begin{aligned}
f(\alpha x + (1-\alpha)y) &= \beta_1 f_1(\alpha x + (1-\alpha)y) + \cdots + \beta_k f_k(\alpha x + (1-\alpha)y) && (12)\\
&\leq \beta_1 \alpha f_1(x) + \beta_1(1-\alpha) f(y) + \cdots + \beta_k \alpha f_k(x) + \beta_k(1-\alpha) f_k(y) && (13)\\
&= \alpha(\beta_1 f_1(x) + \cdots + \beta_k f_k(x)) + (1-\alpha)(\beta_1 f_1(y) + \cdots + \beta_k f_k(y)) && (14)\\
&= \alpha f(x) + (1-\alpha) f(y) && (15)
\end{aligned}
$$

Convexity of MSE

- The mean-squared error is

$$L = \sum_{i=1}^{n} (w^\top x_i - y_i)^2 = \|Xw - y\|_2^2. \tag{16}$$

- We know that the squared distance is convex.
- Use the affine transform and nonnegative weighted sum to obtain the mean-squared error.

Optimality condition

If f is convex and

$$\nabla f(x^*) = 0 \tag{17}$$

at x^*, then x^* is the minimizer of f.

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Proof: Suppose $\nabla f(x^*) = 0$. For any x,

$$f(x) \geq f(x^*) + (x - x^*)^\top \nabla f(x^*) = f(x^*). \tag{18}$$

Optimal solution of MSE

- The mean-squared error is

$$L = \sum_{i=1}^{n} (w^\top \phi(x_i) - y_i)^2 = \|Xw - y\|_2^2. \tag{19}$$

- The solution to $\nabla_w L = 0$ is $w^* = (X^\top X)^{-1} X^\top y$.

- Because L is convex in w, w^* is a minimizer of L.

Convexity of log loss

- The log loss in the binary case is

$$L = \sum_{i=1}^{N} \log\left(1 + \exp(-y_i w^\top x_i)\right). \tag{20}$$

- We just need to show $\ell(s) = \log(1 + \exp(-s))$ is convex in s.

- Use affine transform and nonnegative weighted sum to obtain the log loss.

$$\frac{\partial \ell}{\partial s} = \frac{-\exp(-s)}{1+\exp(-s)} = \frac{1}{1+\exp(-s)} - 1 \tag{21}$$

$$\frac{\partial^2 \ell}{\partial s^2} = \frac{1}{1+\exp(-s)} \frac{\exp(-s)}{1+\exp(-s)} = \frac{1}{1+\exp(-s)}\left(1 - \frac{1}{1+\exp(-s)}\right) \geq 0 \tag{22}$$

Strictly convex functions

A function f is **strictly convex** if

$$f(\alpha x + (1-\alpha)y) < \alpha f(x) + (1-\alpha) f(y), \tag{23}$$

for every $x \neq y$, and $0 \leq \alpha \leq 1$.

Properties of strictly convex functions

- If f is strictly convex, then

$$f(x) > f(y) + \nabla f(y)^\top (x - y), \tag{24}$$

for any $x \neq y$.

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- If f is strictly convex, then

$$f(x) > f(y) + \nabla f(y)^\top (x - y), \tag{24}$$

  for any $x \neq y$.

- A matrix H is positive definite if $v^\top H v > 0$ for any $v \neq 0$.

- If the Hessian of f is positive definite, then f is strictly convex.

Uniqueness of minimizers for strictly convex functions

A strictly convex function f has a unique minimizer.

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A strictly convex function f has a unique minimizer.

Proof: Suppose x^* is a minimizer of f, i.e., $\nabla f(x^*) = 0$. Since f is strictly convex,

$$f(x) > f(y) + \nabla f(y)^\top (x - y) \tag{25}$$

for any $x \neq y$. In particular, if we let $y = x^*$