Fundamentals of Learning and Information Processing

Session 16: Statistical Machine Learning (VI)

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Convex Optimisation

Convexity

A set C in a vector space is convex if for any two vectors $\mathbf{u}, \mathbf{v} \in C$, the line segment between $\mathbf{u}$ and $\mathbf{v}$ is contained in C. Namely, for any $\alpha \in [0,1]$ we have the convex combination $\alpha\mathbf{u} + (1-\alpha)\mathbf{v}$ is in C

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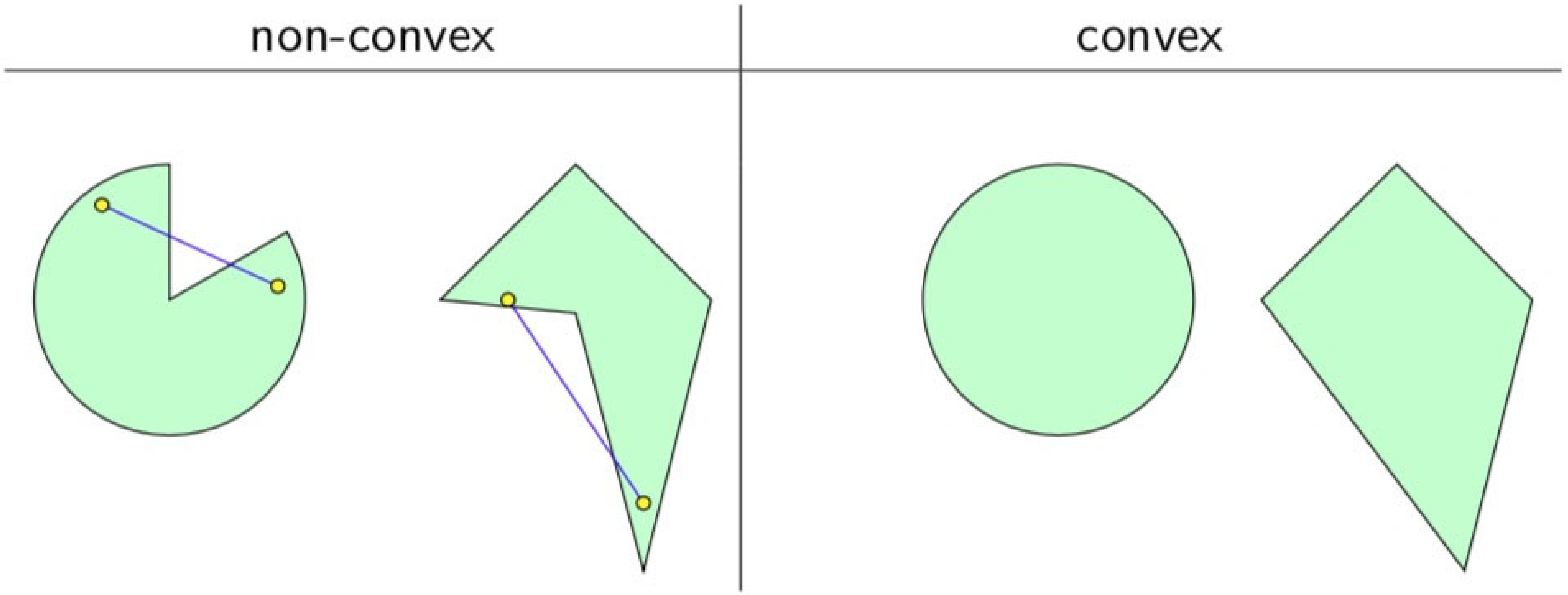

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Let set C be a convex set. A function $f : C \mapsto \mathbb{R}$ is convex if for any two vectors $\mathbf{u}, \mathbf{v} \in C$ and $\alpha \in [0, 1]$,

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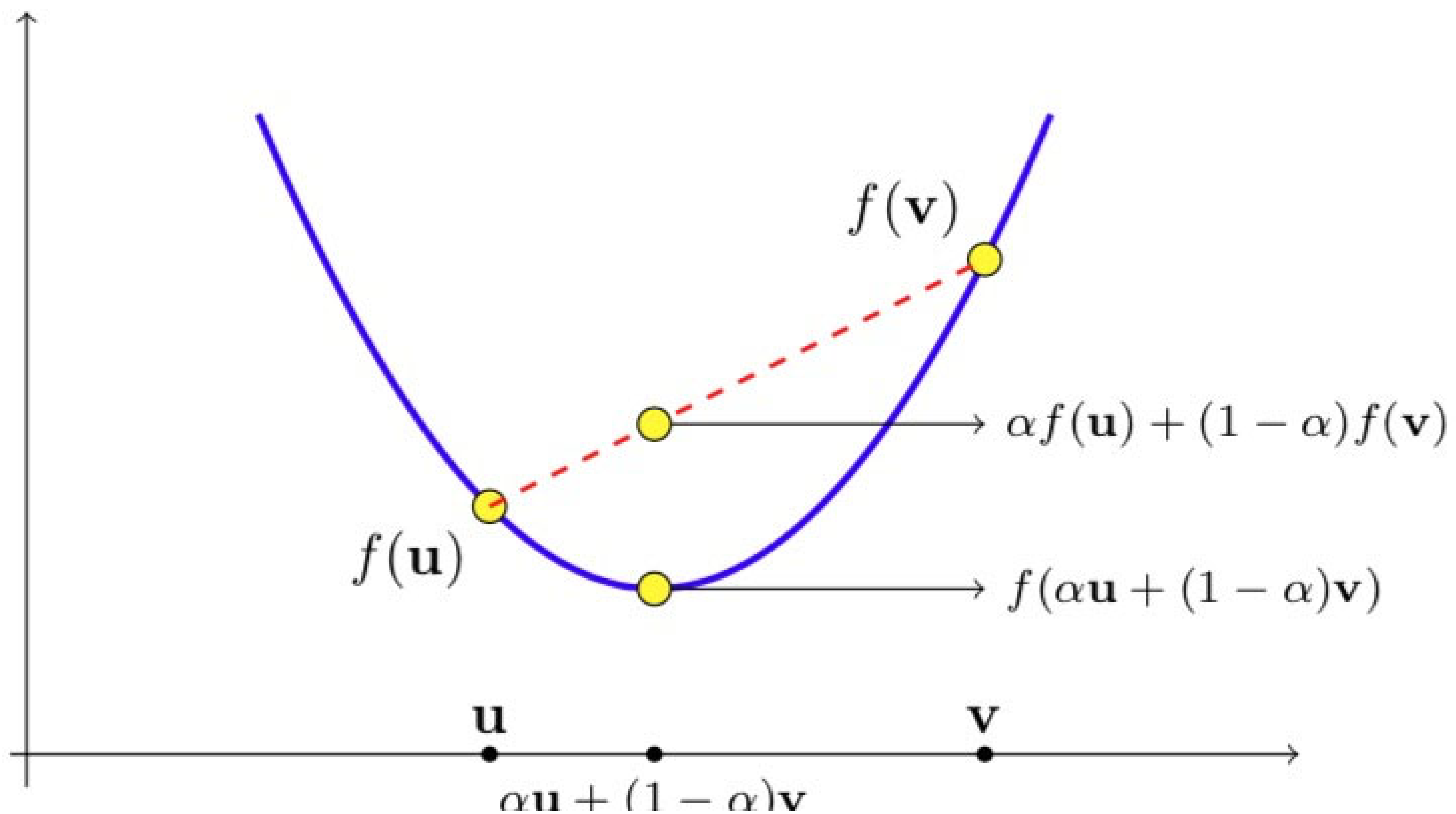

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A function f is convex if and only if its epigraph is a convex set:

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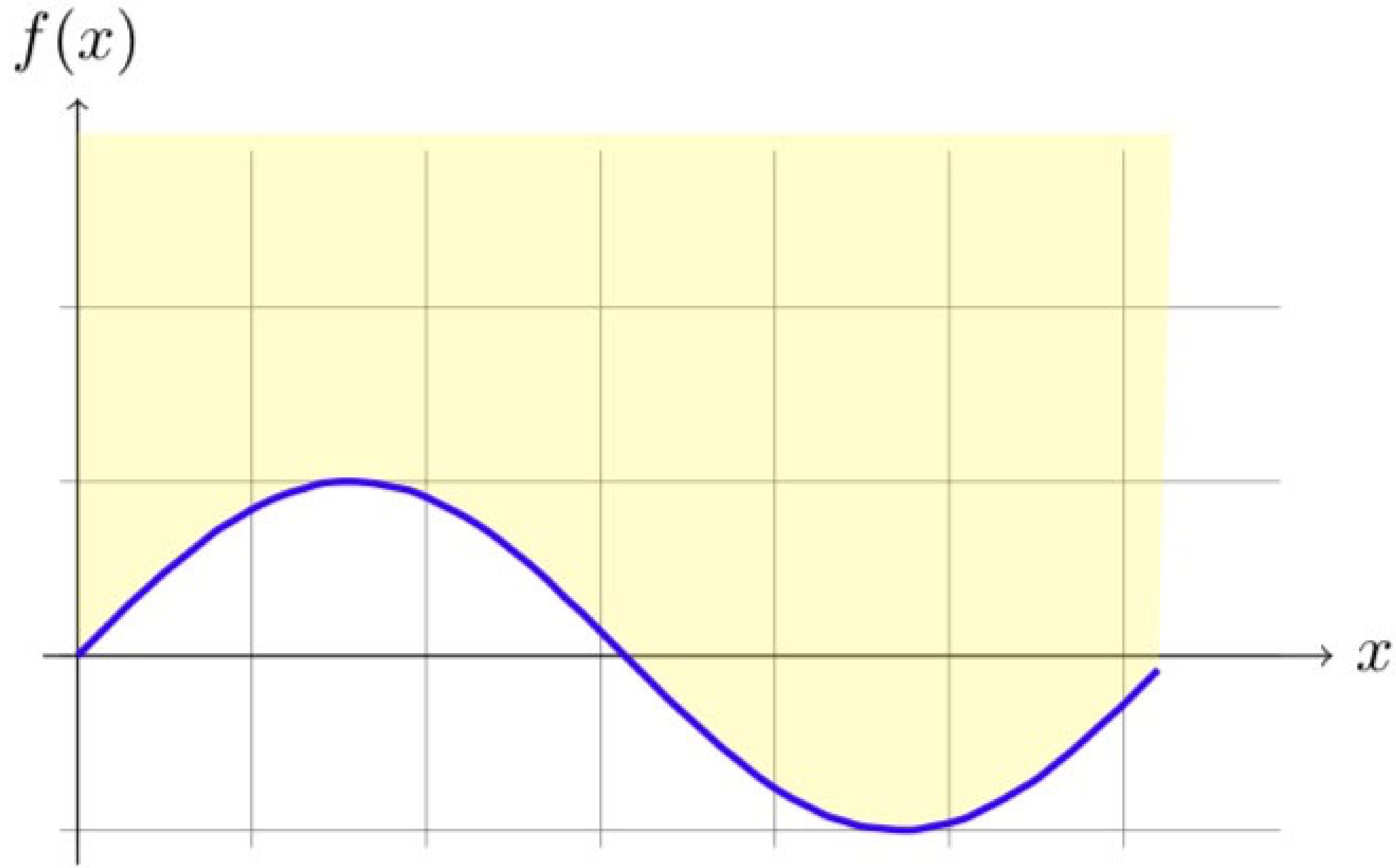

Properties of Convexity (I)

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- It follows that for any v (not necessarily in B), there is a small enough $\alpha > 0$ such that $u + \alpha(v - u) \in B(u,r)$ and therefore

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If a function f is convex and differentiable, then

$$\forall \mathbf{u}, f(\mathbf{u}) \geq f(\mathbf{w}) + \langle \nabla f(\mathbf{w}), \mathbf{u} - \mathbf{w} \rangle$$

- $\nabla f(\mathbf{w}) = (\frac{\partial f(\mathbf{w})}{\partial \omega_1}, \cdots, \frac{\partial f(\mathbf{w})}{\partial \omega_d})$ is the gradient of f at $\mathbf{w}$
- A vector $\mathbf{v}$ is a sub-gradient of f at $\mathbf{w}$ if $\forall \mathbf{u}$, $f(\mathbf{u}) \geq f(\mathbf{w}) + \langle \mathbf{v}, \mathbf{u} - \mathbf{w} \rangle$
- The set of sub-gradients of f at $\mathbf{w}$ is called the differential set, $\partial f(\mathbf{w})$.
    - f is convex if and only if for every $\mathbf{w}$, $\partial f(\mathbf{w}) \neq \emptyset$
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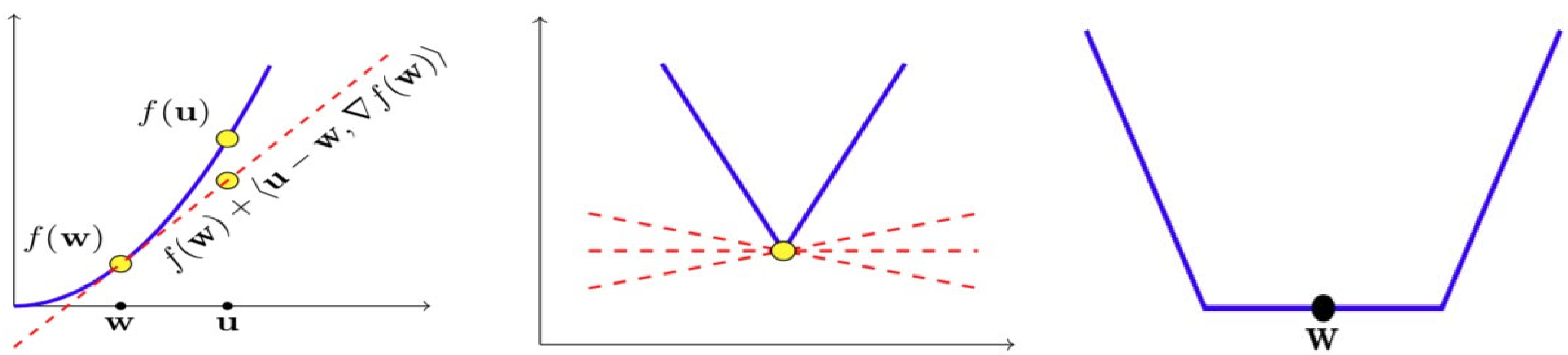

Properties of Convexity (III)

Let f be a scalar twice differential function, and let f', f'' be its first and second derivatives, respectively, then the following are equivalent

- f is convex
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  - Assume that $f : \mathscr{R}^d \mapsto \mathscr{R}$ can be written as $f(\mathbf{w}) = g(\langle \mathbf{w}, x\rangle + y)$, for some $\mathbf{x} \in \mathscr{R}^d$, $y \in \mathscr{R}$ and $g : \mathscr{R} \mapsto \mathscr{R}$. Then the convexity of g implies the convexity of f.

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- The maximum of convex functions is convex and that a weighted sum of convex functions, with non-negative weights, is also convex.
  - For $i = 1, \ldots, r$, let $f_i : \mathscr{R}^d \mapsto \mathscr{R}$ be a convex function. The following functions from $\mathscr{R}^d$ to $\mathscr{R}$ are also convex:
    - $g(x) = \max_{i \in [r]} f_i(x)$
    - $g(x) = \sum_{i=1}^{r} \omega_i f_i(x)$, where $\forall i$, $\omega_i \geq 0$.

Lipschitzness

A function $f : C \mapsto \mathscr{R}$ is ρ-Lipschitz if for every $\omega_1, \omega_2 \in \mathscr{R}$, we have that

$$|f(\omega_1) - f(\omega_2)| \leq \rho \|\omega_1 - \omega_2\|$$

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Examples.

- The linear function $f(\omega) = \langle v, \omega \rangle + b$, where $v \in \mathscr{R}^d$ is $\|v\|$-Lipschitz, from the Cauchy-Schwatz inequality:

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- A Lipschitzness function cannot change too fast: if a Lipschitzness function f is differentiable, then its derivative is everywhere bounded by ρ.
- Let $f(x) = g_1(g_2(x))$, where g_1 is ρ_1-Lipschitz and g_2 is ρ_2-Lipschitz. Then f is $\rho_1 \rho_2$-Lipschitz.

□

Smoothness

A differentiable function $f : C \mapsto \mathscr{R}$ is β-smooth if its gradient is β-Lipschitz; namely, for all ω_1, ω_2 we have

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- Smoothness implies that for all v and ω,

$$f(v) \leq f(\omega) + \langle \triangledown f(\omega), v - \omega \rangle + \frac{\beta}{2} \|v - \omega\|^2$$

Recall that convexity implies that $f(v) \geq f(\omega) + \langle \triangledown f(\omega), v - \omega \rangle$. Therefore, when a function is both convex and smooth, we have both upper and lower bounds on the difference between the function and its first order approximation.

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- Setting $v = \omega - \frac{1}{\beta} \bigtriangledown f(\omega)$, we have $\frac{1}{2\beta} \|\bigtriangledown f(\omega)\|^2 \leq f(\omega) - f(v)$. When $f(v) \geq 0$, we have $\|\bigtriangledown f(\omega)\|^2 \leq 2\beta f(\omega)$, a function satisfying this property is called self-bounded function.

$\square$

Convex Optimization Algorithms

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Approximately solve the problem of

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where C is a convex set and f is a convex function

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  - Adding the constraint $f(\omega) \leq f^* + \epsilon$ eliminates the objective

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Gradient Descent: first-order method

To minimize a differentiable convex function $f(\omega)$, assume the gradient of $f:\mathscr{R}^d \longmapsto \mathscr{R}$ at ω, denoted as $\nabla f(\omega) = (\frac{\partial f(\omega)}{\partial \omega_1}, \cdots, \frac{\partial f(\omega)}{\partial \omega_d})$ is the gradient of f at ω.

- Start with initial $\omega^{(1)}$ (usually, the zero vector)
- At iteration t, update $\omega^{(t+1)} = \omega^{(t)} - \eta \nabla f(\omega^{(t)})$ where η is the learning rate.
- Sub-gradient Descent: for non differentiable function f, we can replace gradients with sub-gradients: update $\omega^{(t+1)} = \omega^{(t)} - \eta v_t$ where $v_t \in \partial f(\omega^{(t)})$.

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- We can minimize the appropriation of $f(\omega)$, but also wish the approximation to be accurate. Therefore, we would like to minimize jointly the distance between ω and $\omega^{(t)}$, and the approximation of f around $\omega^{(t)}$. If η controls the trade-off between those two terms, we obtain the update rule:

$$\omega^{(t+1)} = \arg\min_{\omega} \frac{1}{2} \|\omega - \omega^{(t)}\|^2 + \eta(f(\omega^{(t)}) + \langle \nabla f(\omega^{(t)}), \omega - \omega^{(t)} \rangle)$$

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Analysing Gradient Descent for Lipschitz functions

To minimize a convex function $f(\omega)$, let ω^* be any vector, which could be the minimizer of $f(\omega)$, and B be an upper bound on $\|\omega^*\|$, namely $\|\omega^*\| \leq B$. We can obtain an upper bound on the suboptimality w.r.t. ω^*: $f(\bar{\omega}) - f(\omega)$, where $\bar{\omega} = \frac{1}{T}\sum_{t=1}^{T} \omega^{(t)}$.

$$f(\bar{\omega}) - f(\omega^*) \leq \frac{1}{T}\sum_{t=1}^{T} \langle \mathbf{v}_t, \omega^{(t)} - \omega^* \rangle \leq \frac{B^2}{2\eta T} + \frac{\eta}{2T}\sum_{t=1}^{T} \|\mathbf{v}_t\|^2$$

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- Followed by the convexity of f, we have $f(\omega^{(t)}) - f(\omega^*) \leq \langle \mathbf{v}_t, \omega^{(t)} - \omega^* \rangle$

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- Summing them together as below: when $\omega^{(1)} = 0$, the previous statement is proved.

$$\begin{aligned}\sum_{t=1}^{T}\langle \mathbf{v}_t, \omega^{(t)} - \omega^* \rangle &= \frac{1}{2\eta}(\|\omega^{(1)} - \omega^*\|^2 - \|\omega^{(T+1)} - \omega^*\|^2) + \frac{\eta}{2}\sum_{t=1}^{T}\|\mathbf{v}_t\|^2 \\ &\leq \frac{1}{2\eta}(\|\omega^{(1)} - \omega^*\|^2) + \frac{\eta}{2}\sum_{t=1}^{T}\|\mathbf{v}_t\|^2\end{aligned}$$

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- Since f is convex and ρ-Lipschitz, $\mathbf{v}_t \le \rho$ for every t. Therefore

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Analysing Gradient Descent for Lipschitz functions

To minimize a convex function $f(\omega)$, let ω^* be any vector, which could be the minimizer of $f(\omega)$, and B be an upper bound on $\|\omega^*\|$, namely $\|\omega^*\| \leq B$. We can obtain an upper bound on the suboptimality w.r.t. ω^*: $f(\bar{\omega}) - f(\omega)$, where $\bar{\omega} = \frac{1}{T}\sum_{t=1}^{T} \omega^{(t)}$.

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- For every ω^*, if $T > \frac{B^2\rho^2}{\epsilon^2}$, and $\eta = \sqrt{\frac{B^2}{\rho^2 T}}$, then the right side is at most ϵ. Hence $f(\bar{\omega}) - f(\omega^*) \leq \epsilon$.
- This indicates that the gradient descendent method needs $\frac{B^2\rho^2}{\epsilon^2}$ steps to converge.

$\square$

Stochastic Gradient Descent (SGD): first-order method

To minimize a differentiable convex-Lipschitz-bounded function $f(\omega)$, the goal is to probably approximately solve $\min_\omega L_{\mathscr{D}}(\omega)$ where $L_{\mathscr{D}}(\omega) = E_{z\sim\mathscr{D}} l(\omega, z)$

- initialize: $\omega^{(1)} = 0$
- for $i = 1, \cdots, T$
  - choose $z_t \sim \mathbb{D}$
  - let $\mathbf{v}_t \in \partial l(\omega^{(t)}, z)$
  - update $\omega^{(t+1)} = \omega^{(t)} - \eta \mathbf{v}_t$
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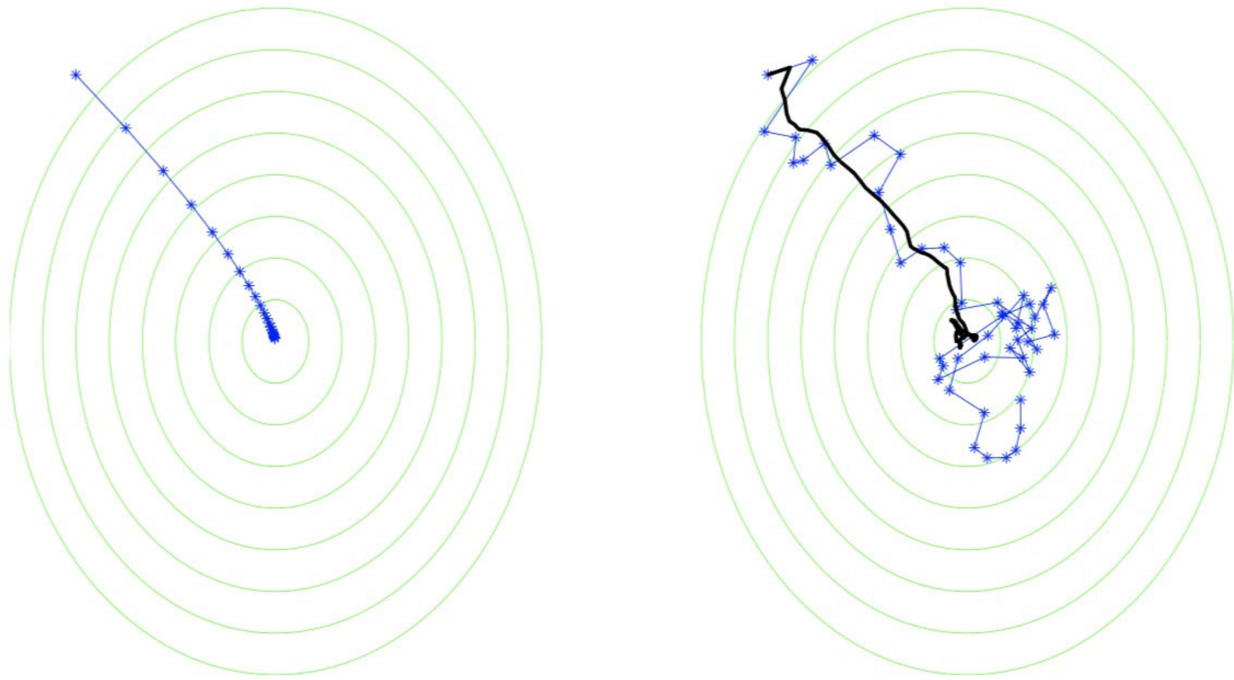

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- We can not calculate $\nabla L_{\mathscr{D}}(\omega^{(t)})$ because we don't know $\mathscr{D}$, but we can estimate it by $\nabla l(\omega, z)$ for $z \sim \mathscr{D}$.
- If we take a step in the direction $\mathbf{v} = \nabla l(\omega, z)$, then in expectation we are moving in the right direction. Namely $\mathbf{v}$ is an unbiased estimate of the gradient.

Consider a convex-Lipschitz-bounded learning problem with parameters ρ, and B be an upper bound on $\|\omega^*\|$. Then, for every $\epsilon > 0$, if we run the SGD method for minimizing $L_{\mathscr{D}}(\omega)$ with a number of iterations (i.e., number of examples) $T \geq \frac{B^2\rho^2}{\epsilon^2}$ and with $\eta = \sqrt{\frac{B^2}{\rho^2 T}}$, then the output of SGD satisfies:

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3. Take expectation of both sides w.r.t. the randomness of choosing $z_1, \cdots z_T$ we obtain: $E_{z_1,\cdots,z_T}[\sum_{t=1}^{T} \langle \mathbf{v}_t, \omega^{(t)} - \omega^* \rangle] \leq B\rho\sqrt{T}$

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8. Divided by T and using convexity again, we have $E_{z_1,\cdots,z_T}[L_{\mathscr{D}}(\frac{\sum_{t=1}^T \omega^{(t)}}{T})] \leq L_{\mathscr{D}}(\omega^*) + \frac{B\rho}{\sqrt{T}}$

$\square$

Newton's method: second-order method

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- For zero finding in $f(\omega)$, Newton's method iterates as:

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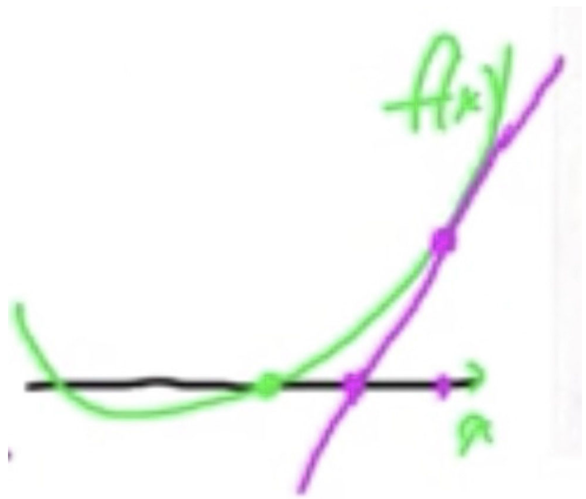

- Finding the minimum or maximum of f is equal to zero finding in function f', hence Newton's method of optimisation iterates as

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Intuition.

- Let f to be sufficiently smooth. By Taylor's approximation, if close to $\omega^{(t)}$, we have

$$
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f(x) &\approxeq f(\omega^{(t)}) + g^T(x - \omega^{(t)}) + \frac{1}{2}(x - \omega^{(t)})^T H (x - \omega^{(t)}) \\
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- Take the first derivative, we have $\nabla f = Hx + (g - H\omega^{(t)}) = 0$. So we have $x = -H^{-1}(g - H\omega^{(t)}) = \omega^{(t)} - H^{-1} g$

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- Because $\nabla^2 f = H$, so f is minimized when H is positive self-definite.

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- Because $\nabla^2 f = H$, so f is minimized when H is positive self-definite.
- H may fail to be positive definite, rather than inverse H, we may solve $Hy = g$ for y, then use $\omega^{(t+1)} = \omega^{(t)} - y$

Newton's method: second-order method

To minimize a twice differentiable convex function $f(\omega)$, assume the gradient of $f : \mathscr{R}^d \mapsto \mathscr{R}$ at ω, denoted as $g = \nabla f(\omega) = (\frac{\partial f(\omega)}{\partial \omega_1}, \cdots, \frac{\partial f(\omega)}{\partial \omega_d})$ is the gradient of f at ω, and the Hessian $H = \nabla^2 f(\omega)$

- Start with initial $\omega^{(1)}$ (usually, the zero vector)
- At iteration t, update $\omega^{(t+1)} = \omega^{(t)} - H^{-1} g$

Properties.

- Because $\nabla^2 f = H$, so f is minimized when H is positive self-definite.
- H may fail to be positive definite, rather than inverse H, we may solve $Hy = g$ for y, then use $\omega^{(t+1)} = \omega^{(t)} - y$
- We may also introduce the learning rate η, hence $\omega^{(t+1)} = \omega^{(t)} - \eta y$

□

Convex Learning Problems

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A learning problem $(\mathcal{H}, \mathcal{Z}, l)$ is called convex if the hypothesis class $\mathcal{H}$ is a convex set and for all $z \in \mathcal{Z}$, the loss function $l(\cdot, z)$ is a convex function, where for any z, $l(\cdot, z)$ denotes the function $f : \mathcal{H} \mapsto \mathcal{R}$ defined by $f(\omega) = l(\omega, z)$.

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Claims.

- $ERM_{\mathcal{H}}$ w.r.t. a convex learning problem is a convex optimization

$$\min_{\omega \in \mathcal{H}} \frac{1}{m} \sum_{i=1}^{m} l(\omega, z_i)$$

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  - The intuitive reason is numerical stability.
- With two additional mild conditions, we obtain learnability.

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Convex-Lipschitz-bounded learning problem

A learning problem $(\mathscr{H}, \mathcal{Z}, l)$ is called convex-Lipschitz-Bounded, with parameters ρ and B if the following holds:

- The hypothesis class $\mathscr{H}$ is a convex set, and $\forall \omega \in \mathscr{H}$ we have $\|\omega\| \leq B$.
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Notes.

- When trying to minimize the empirical risk with respect to a non convex loss function, we might encounter local minima.
- Also solving the ERM problem with respect to the $0-1$ loss in the unrealisable case is known to be NP-hard.

□

The $0-1$ Loss Function and Hinge Loss

In the context of learning halfspaces, the $0-1$ loss is not convex:

$$l^{0-1}(\omega,(x,y)) = 1_{y \neq sign(\langle \omega, x \rangle)} = 1_{y\langle \omega, x \rangle \leq 0}$$

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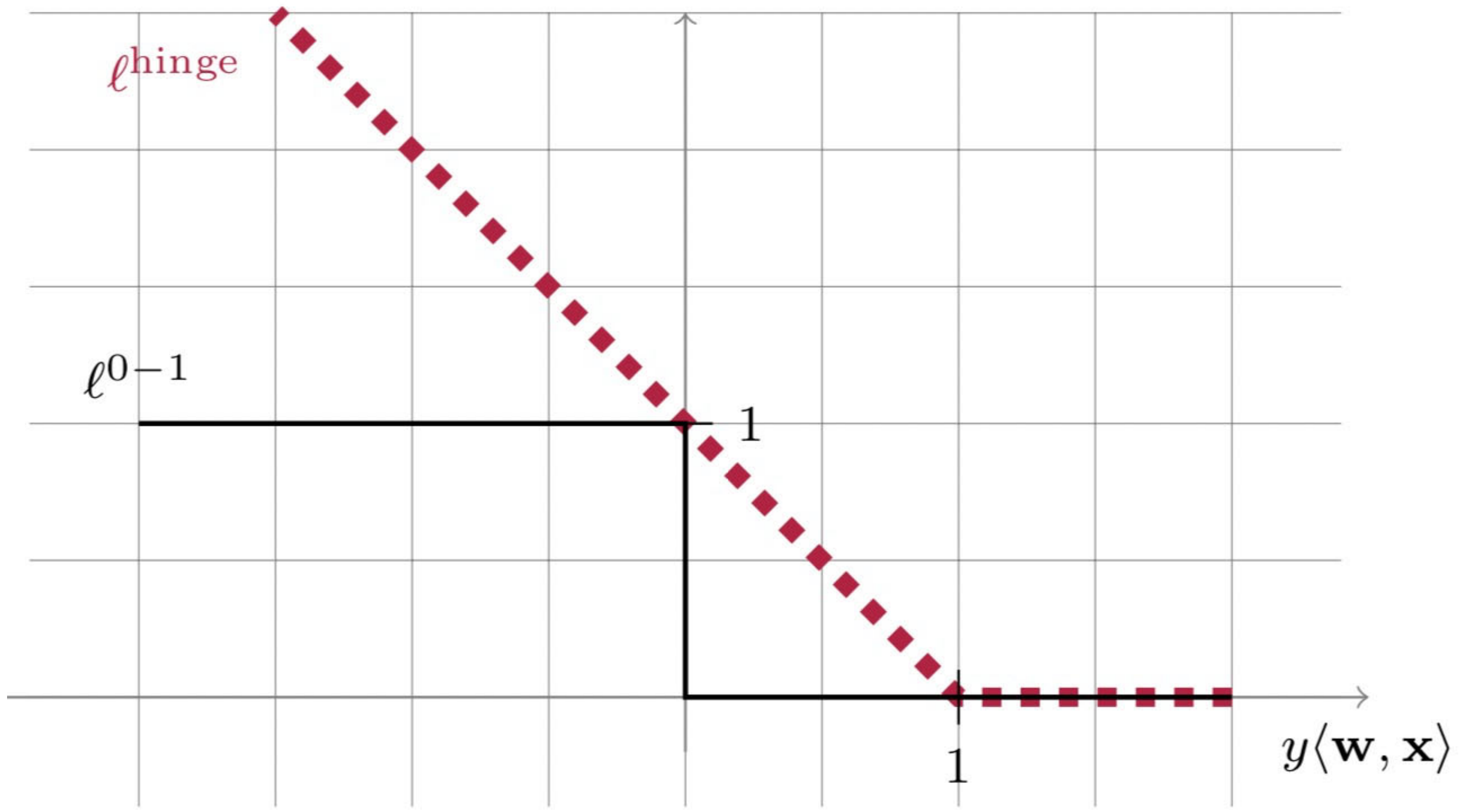

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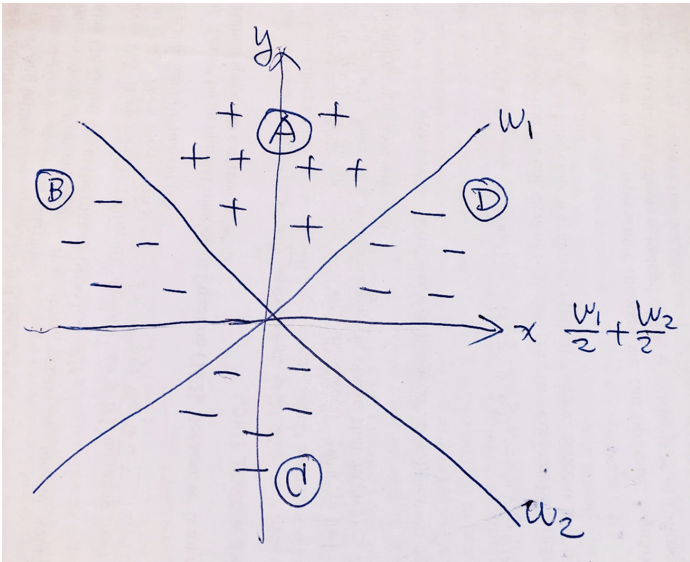
- Hence it is non-convex.



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  - We can see $\langle \omega, x\rangle = \langle \omega_x, \vec{v}\rangle + \omega_0 = \langle \omega_x, \vec{x}\rangle - (\langle \omega_x, \vec{x}\rangle + \omega_0)\|\omega_x\|^2 + \omega_0 = 0$

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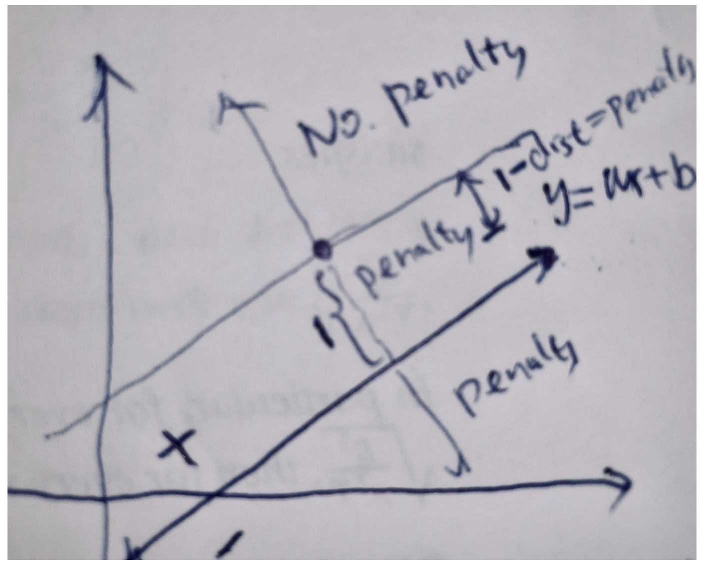
- Geometrically, l^{hinge} represents the penalty or loss which considers the margin of the classifier:
  - No penalty for corrected examples larger than the margin
  - $1 - y\langle \omega, x \rangle$ for corrected examples within the margin, or wrong examples



Error Decomposition Revisited

Suppose we have a learner for the hinge-loss that guarantees: $L_{\mathscr{D}}^{hinge}(A(S)) \leq \min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{hinge}(\omega) + \epsilon$. Using the surrogate, we have $L_{\mathscr{D}}^{0-1}(A(S)) \leq \min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{hinge}(\omega) + \epsilon$. We can further rewrite the upper bound as:

$$l^{0-1}(A(S)) \leq \min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{0-1}(\omega) + (\min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{hinge}(\omega) - \min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{0-1}(\omega)) + \epsilon$$

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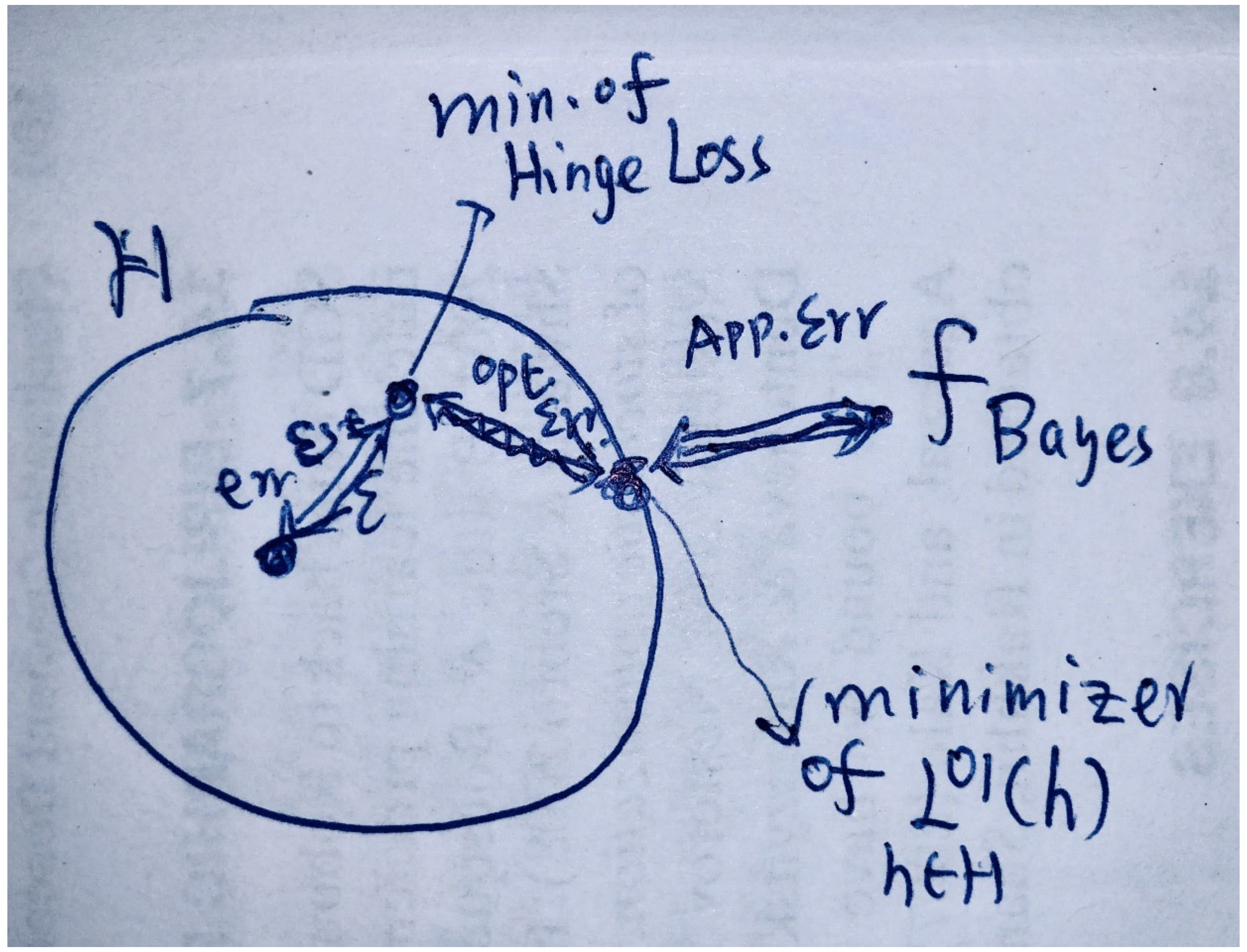

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Optimisation Error $(\min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{hinge}(\omega) - \min_{\omega\in\mathbb{H}} L_{\mathscr{D}}^{0-1}(\omega))$ which measures the difference between the approximation error with respect to the surrogate loss and the approximation error with respect to the original loss.

- It is the result of our inability to minimize the training loss with respect to the original loss.
- Its size depends on the specific data distribution and on the specific surrogate loss.

Quiz

SGD with Projection Step

In the SGD or GD, the norm of ω is required to be at most B. But there is no guarantee that ω in SGD/GD will satisfy it.

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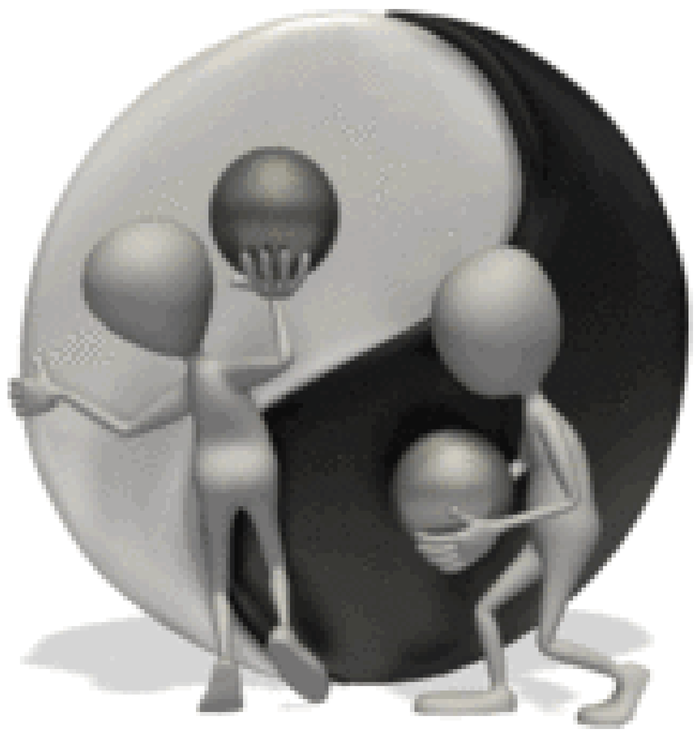
  The project step replaces the current value of ω by the vector in $\mathcal{H}$ closest to it.
- Projection Lemma: Let $\mathcal{H}$ be a closed convex set, and let v be the projection of ω onto $\mathcal{H}$, namely, $v = \arg\min_{x \in \mathcal{H}} |x - \omega|^2$. Then prove that: for every $u \in \mathcal{H}$, $|\omega - u|^2 - |v - u|^2 \geq 0$.

Questions?



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