The duality between maximum separation and minimum distance

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[1] Joint work with Peter Gritzmann and Thomas Burger

Outline

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Margin

Definition

Given $P, Q \subset \mathbb{R}^d$, $f : \mathbb{R}^d \to \mathbb{R}$ *classifies* P and Q with *margin* γ if

$$\gamma = \inf_{p \in P} f(p) - \sup_{q \in Q} f(q) = \inf_{p \in P, q \in Q} f(p) - f(q)$$

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Roughly speaking

We want to maximize γ/γ^*, where γ^* is a *best possible margin* for some family $\mathcal{F} \ni f$

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Toy example

- $P, Q \subset [0, 1]$
- $\mathcal{F} = \{x \to x, x \to -x\}$
- $\gamma^* = 1$

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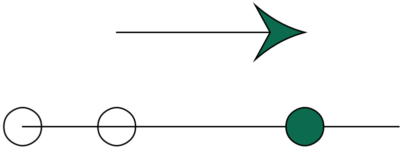

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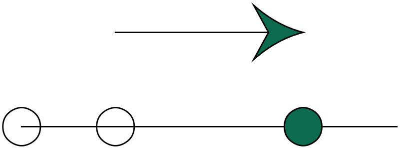

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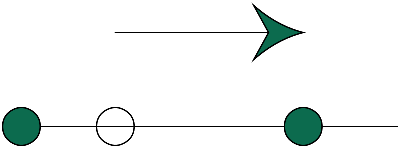

$\gamma = -1/4$

Linear Classifiers and Support Functionals

Linear Classifiers

$$f(x) = \langle z, x \rangle := \sum_{i=1}^{n} z_i x_i$$

Support Functionals

For $K \subset \mathbb{R}^d, w \in (\mathbb{R}^d)^*$,

$$\sup(K; w) := \sup_{k \in K} \langle w, k \rangle \qquad \text{(upper)}$$

$$\inf(K; w) = \inf_{k \in K} \langle w, k \rangle \qquad \text{(lower)}$$

$$= -\sup(K; -w)$$

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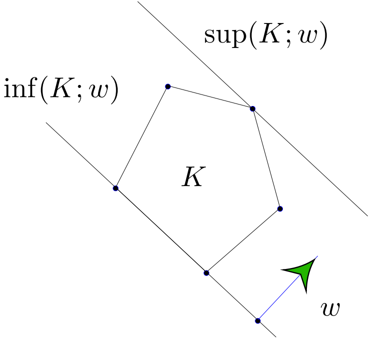

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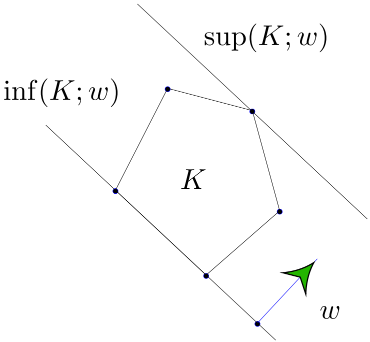

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W.l.o.g, K is convex

$$\sup(X; w) = \sup(\text{conv}(X); w)$$

Linear Margin

Margin optimization

$$\max \inf(P; z) - \sup(Q; z) \quad \text{such that}$$
$$z \in (\mathbb{R}^d)^*$$

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If $\inf(P; z) - \sup(Q; z) = \gamma$ then for $\tau \geq 0$,

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Scaling up

So that margin(P, Q) is not always $+\infty$, $z \in \mathbb{B}^*$, $\mathbb{B}^*$ bounded.

Linear Margin

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$$\max \inf(P; z) - \sup(Q; z) \quad \text{such that}$$
$$z \in \quad \mathbb{B}^* \setminus L$$

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Scaling down

For some region $\vec{0} \in L \subset \mathbb{B}^*$, $z \notin L$

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Without much loss of generality

- W.l.o.g. $\mathbb{B}^*$ is a *convex body*, i.e. convex, has interior.
- It seems natural then to choose $L = \operatorname{int} \mathbb{B}^*$.

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Minkowski Norms

- $X \subset \mathbb{R}^d$ is *centrally symmetric* if $x \in X \Rightarrow -x \in X$.
- For any centrally symmetric convex body $\mathbb{B}$, the *Minkowski Norm*

$$\|x\|_{\mathbb{B}} := \inf_{\lambda \geq 0} \{ \lambda \geq 0 \mid x \in \lambda \mathbb{B} \}$$

- For any $K \subset \mathbb{R}^d$, the *polar* $K^* = \{ y \in \mathbb{R}^n \mid \sup(K; y) \leq 1 \}$.

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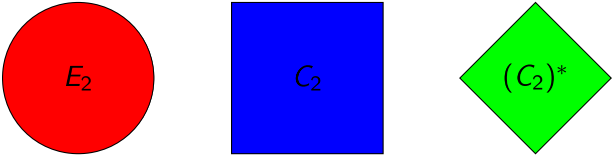

$\|\cdot\|_2 = \sqrt{x_1^2 + x_2^2}$ $\quad$ $\|\cdot\|_\infty = \max(|x_1|, |x_2|)$ $\quad$ $\|\cdot\|_1 = |x_1| + |x_2|$

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- Choose $z \in \operatorname{bd} \mathbb{B}^*$

$$\begin{aligned} \max \inf(P; z) - \sup(Q; z) \\ z \in \mathbb{S}^* \end{aligned}$$

Norm duality

Polarity of unit balls connects norms:

$$\|x\|_{\mathbb{B}} = \sup(\mathbb{B}^*; x) \tag{ND}$$

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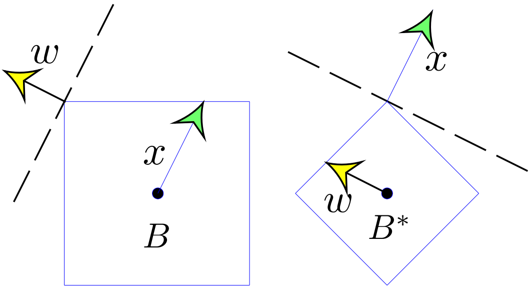

Norms define metrics

- Define

$$\mathrm{dist}_{\mathbb{B}}(x, y) := \|x - y\|_{\mathbb{B}}$$
$$\mathrm{dist}_{\mathbb{B}}(X, Y) := \inf_{x \in X, y \in Y} \|x - y\|_{\mathbb{B}}$$
$$H(z, \varphi) = \{\, x \in \mathbb{R}^n \mid \langle\, z, x \,\rangle = \varphi \,\}$$

- Where $\mathbb{B}$ is clear from context, we write $\|\cdot\|$, and $\mathrm{dist}(\cdot, \cdot)$.
- From (ND), we have for all $z \in \mathbb{S}^*$,

$$\mathrm{dist}(H(z, \mu_1), H(z, \mu_2)) = |\mu_1 - \mu_2| \tag{1}$$

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Separability

Separable

$P, Q \subset \mathbb{R}^d$ are *separable* if $\exists z \neq \vec{0}$ such that $\sup(Q; z) \leq \inf(P; z)$.

Theorem (The Separating Hyperplane Theorem)

Given convex sets P and Q with $\operatorname{aff}(P \cup Q) = \mathbb{R}^d$, $\operatorname{relint} S \cap \operatorname{relint} T \neq \emptyset$ *if and only if P and Q are not separable.*

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Corollary

For P, Q convex polyhedra, $\operatorname{sep}(P, Q)$ *is computable in polynomial time.*

Margin as distance between parallel hyperplanes

Dual Unit Ball Formulation

$$\max \inf(P; z) - \sup(Q; z)$$
$$z \in \mathbb{S}^*$$

Parallel Hyperplane Distance

$$\max \operatorname{sep}(P, Q) \cdot \operatorname{dist}(H(z, \inf(P; z)), H(z, \sup(Q; z)))$$
$$z \neq \vec{0}$$

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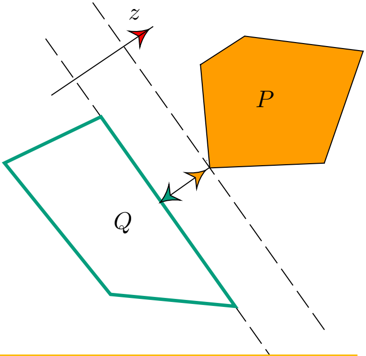

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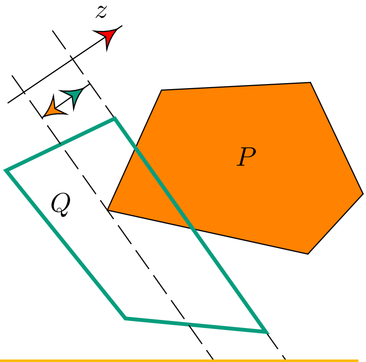

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The *Minkowski sum* and *Minkowski difference* of $P, Q \subset \mathbb{R}^n$ is defined as

$$P + Q = \{\, x + y \mid x \in P \text{ and } y \in Q \,\}$$
$$P - Q = P + (-Q) = \{\, x - y \mid x \in P \text{ and } y \in Q \,\}$$

Support is Minkowski-additive

$$\sup(P + Q; w) = \sup(P; w) + \sup(Q; w) \tag{2}$$

Define $\operatorname{margin}(P, Q)$ as the optimal value of

$$\max \inf(P - Q; w) \quad w \in \mathbb{S}^* \tag{MARGIN}$$

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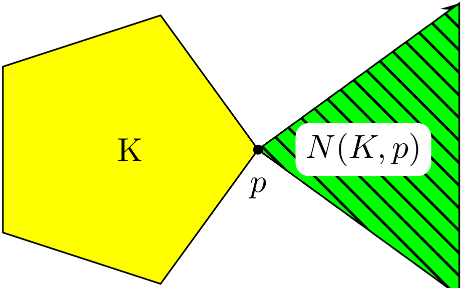
Outer Normal Cones

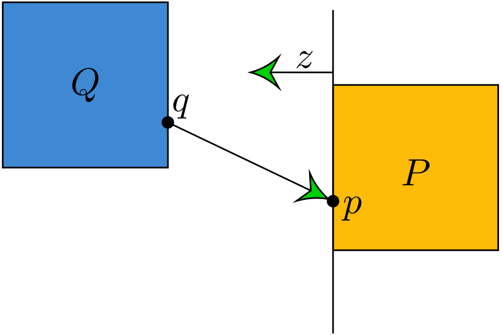
For a convex set $K \subset \mathbb{R}^n$ and a point $x \in K$ the *outer normal cone* of K at x is defined as

$$N(K, x) := \{ z \in (\mathbb{R}^d)^* \mid \langle z, x \rangle = \sup(K; z) \}.$$



Margin by translation

$$\begin{aligned} \min \quad & \|p - q\| \\ \sup(P; z) = & \inf(Q + (p - q); z) \\ z \neq \vec{0}, \quad & q \in Q, \quad p \in P \end{aligned} \tag{3}$$



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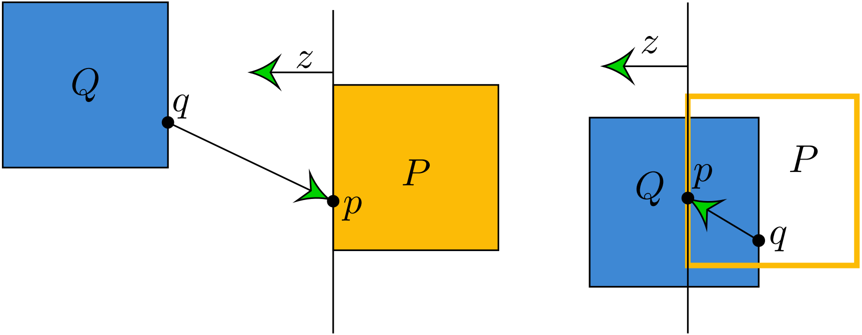

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- Minkowski additivity of support, twice.
- $\vec{0} \neq z \in N(K, r)$ iff $r \in \operatorname{bd} K$.

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Define shift(P, Q) as the solution to the following

$$\begin{aligned} & \min \|r\| \\ & r \in \operatorname{bd} P - Q \end{aligned} \tag{NORM}$$

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Proposition

For convex polyhedra P and Q, $\text{shift}(P, Q)$ is computable in polynomial time given a polynomial sized facet representation for $P - Q$

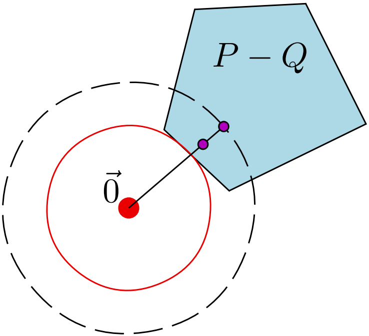
Outline

Finding the minimum translation in the separable case

Proposition

Let P, Q be convex bodies. If $\vec{0} \notin \mathrm{int}(P - Q)$, then

$$\mathrm{shift}(P, Q) = \min_{r \in \mathrm{bd}(P-Q)} \|k\| = \min_{r \in (P-Q)} \|k\|$$



Relaxing (MARGIN)

Proposition

Let P and Q be separable convex bodies.

$$\sup_{w \in \mathbb{S}^*} \inf(P - Q, w) = \sup_{w \in \mathbb{B}^*} \inf(P - Q, w)$$

Proof.

Let $w' := \operatorname{argmax}_{w \in \mathbb{B}^*} \inf(P - Q; w)$.

$$0 \leq \inf(P - Q; w')$$

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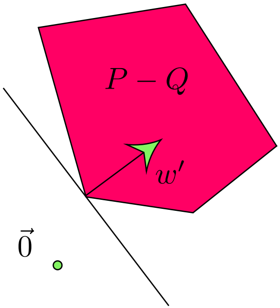

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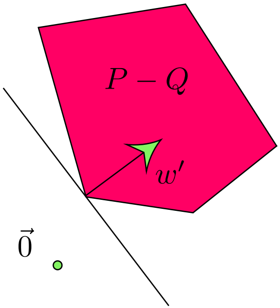

Weak Duality

Proposition

Let $r \in P - Q$, $z \in \mathbb{B}^*$

$$\|r\| \geq \inf(P - Q; z) \tag{4}$$

Proof.

Since $z \in \mathbb{B}^*$, from (ND),

$$\|r\| = \sup(\mathbb{B}^*; r) \geq \langle z, r \rangle \geq \inf(P - Q; z)$$

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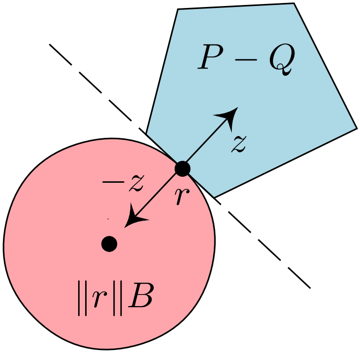
Duality of convex relaxations

Theorem

Let P and Q be separable convex bodies. Vectors $r \in P - Q$ and $z \in \mathbb{B}^*$ form a primal–dual optimal pair for (MARGIN) *and (NORM) iff*

$$\|r\|_{\mathbb{B}} = \langle z, r \rangle \qquad -z \in N(P - Q, r)$$



Skip proof

Necessity

Duality of convex relaxations

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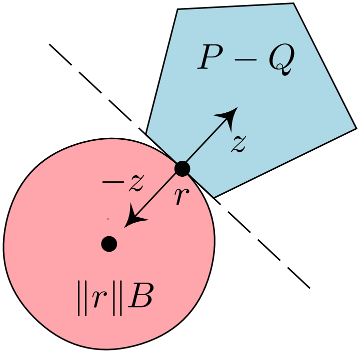

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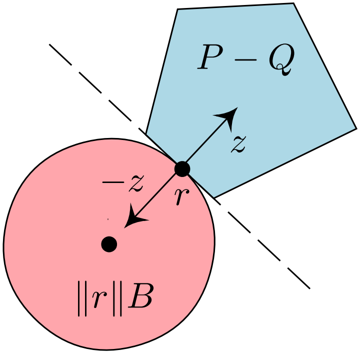
Duality of convex relaxations



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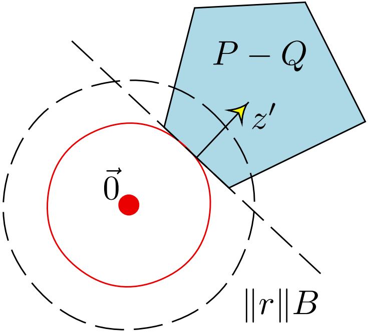
- int $\|r\|\mathbb{B} \cap (P - Q) = \emptyset$



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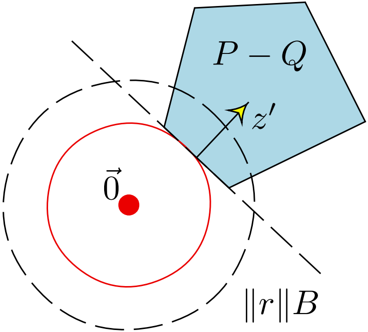
- $\operatorname{int} \|r\|\mathbb{B} \cap (P - Q) = \emptyset$
- By optimality of z,

$$\begin{aligned} \inf(P - Q; z') &\leq \inf(P - Q; z) \\ &\leq \langle z, r \rangle \end{aligned}$$



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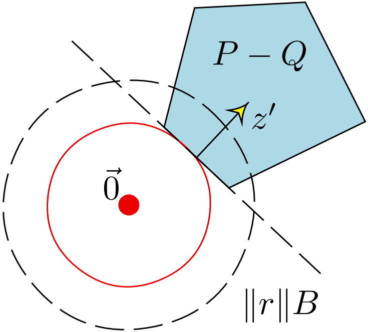
- Now apply Weak Duality.



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Outline

Width of convex bodies

For convex body K, define

$$\text{length}_s(K) := \sup \{\, \tau \mid [x, x + \tau s] \subset K \,\}$$
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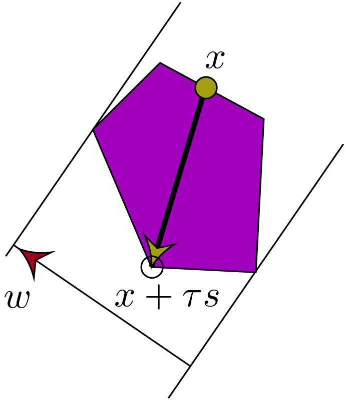

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$$\text{width}(X) := \inf_{w\in\mathbb{S}^*} \text{breadth}_w(X) = \inf_{s\in\mathbb{S}} \text{length}_s(X)$$

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$$\text{width}(X) = -\text{margin}(X, X)$$

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Computing Width is NP-Hard

Theorem (Gritzmann–Klee 1992)

Computing width(K) *is NP-hard, for* K *a simplex, in at least the* L_2 *and* L_∞ *norms.*

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Corollary (GK92, new proof)

Computing width$(\cdot)$ *is solvable in polynomial time for centrally symmetric polytopes given by their facets.*

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For convex body K with $\vec{0} \in K$,

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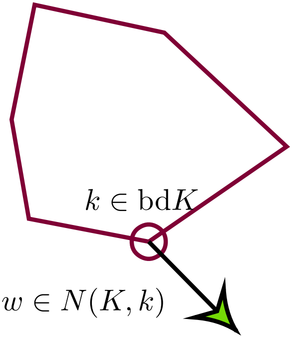

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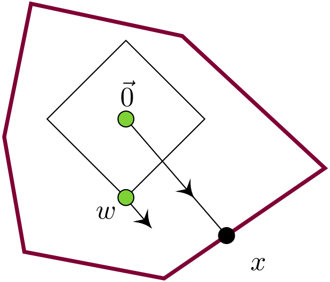
- $\forall w \in \mathbb{S}^* \; \exists x \in N(\mathbb{B}^*, w) \cap \operatorname{bd} K$

  $$\sup(K; w) \geq \langle\, x, w \,\rangle = \|x\|$$



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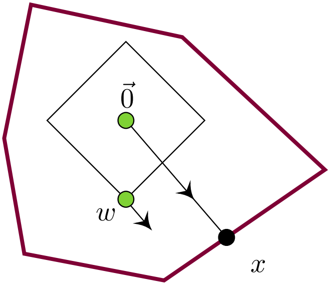
$\operatorname{shift}(P, Q) = -\operatorname{margin}(P, Q)$



Outline

Margin: separation quantified

Margin as a metric problem

A dual formulation via norm minimization

The separable (convex) case

The inseparable case

Conclusions

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$$\mathrm{shift}(P, Q) = \mathrm{sep}(P, Q) \cdot \mathrm{margin}(P, Q)$$

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