Breaking the Curse of Dimensionality with Convex Neural Networks

Francis Bach

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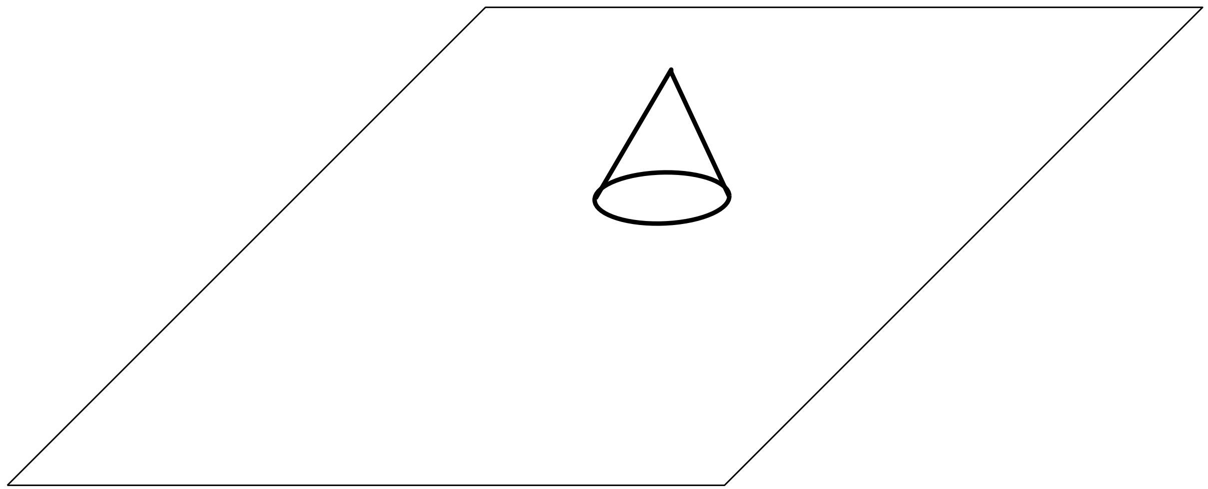
Curse of dimensionality (supervised learning)

- **Goal**: Learning a function $f : \mathbb{R}^d \to \mathbb{R}$ with minimal risk

$$R(f) = \mathbb{E}\big[\ell(y, f(x))\big]$$

  - Minimizer f^* only assumed to be Lipshitz-continuous
  - Need $n = \Omega(\varepsilon^{-d})$ observations to achieve $R(f) - R(f^*) \leqslant \varepsilon$



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- **Reducing sample complexity by exploiting structure**

Linear function	$w^\top x + b$	$d\varepsilon^{-2}$
Generalized additive model	$\sum_{j=1}^{d} f_j(x_j)$	$k^4 d^2 \varepsilon^{-4}$
One-hidden layer neural network	$\sum_{i=1}^{k} \eta_i \sigma(w_i^\top x + b)$	$k^2 d \varepsilon^{-2}$
Projection pursuit	$\sum_{i=1}^{k} f_i(w_i^\top x)$	$k^4 d^2 \varepsilon^{-4}$
Subspace dependence	$g(W^\top x)$	$(\frac{\varepsilon}{k\sqrt{d}})^{-\mathrm{rank(W)}+3}$

Goals

$$f(x) = \sum_{i=1}^{k} \eta_i \max\{w_i^\top x + b_i, 0\} = \sum_{i=1}^{k} \eta_i (w_i^\top x + b_i)_+$$

- **Generalization properties?**
  - Adaptivity to structure
  - Non-linear variable selection

- **Learning or sampling weights** $(w_i, b_i) \in \mathbb{R}^{d+1}$**?**
  - Convexification by letting $k \to +\infty$
  - Selection (ℓ_1) vs. random sampling (ℓ_2)

- **Hard or easy to optimize?**
  - Polynomial time algorithms ...
  - ... with same guarantees on unseen data

Convex neural networks (Bengio, Le Roux, Vincent, Delalleau, and Marcotte, 2006)

Main idea

- **Replace the sum** $\sum_{i=1}^{k} \eta_i (w_i^\top x + b_i)_+$ **by an integral**

$$f(x) = \int_{\mathbb{R}^{d+1}} (w^\top x + b)_+ \, \eta(w,b) d\tau(w,b)$$

  – Equivalence when $\eta d\tau$ is a weighted sum of Diracs: $\sum_{i=1}^{k} \eta_i \delta_{w_i,b_i}$

- **Promote sparsity with an** ℓ_1**-norm**: $\int_{\mathbb{R}^{d+1}} |\eta(w,b)| d\tau(w,b)$

Convex neural networks
Formalization

- **Several points of views** (Barron, 1993; Kurkova and Sanguineti, 2001; Bengio et al., 2006; Rosset et al., 2007)

- Define **space** $\mathcal{F}_1$ **of functions** f that can be decomposed as

$$f(x) = \int_{\mathbb{R}^{d+1}} (w^\top x + b)_+ \; \eta(w,b) d\tau(w,b) \qquad (\bullet)$$

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- Define the **variation norm** $\gamma_1(f)$ on $\mathcal{F}_1$ as

$$\gamma_1(f) = \inf \int_{\mathbb{R}^{d+1}} |\eta(w,b)| d\tau(w,b) \quad \text{such that } (\bullet) \text{ holds}$$

Variation norm and finite decomposition

- **Property 1** (Leshno et al., 1993): $\mathcal{F}_1$ is dense in L^2

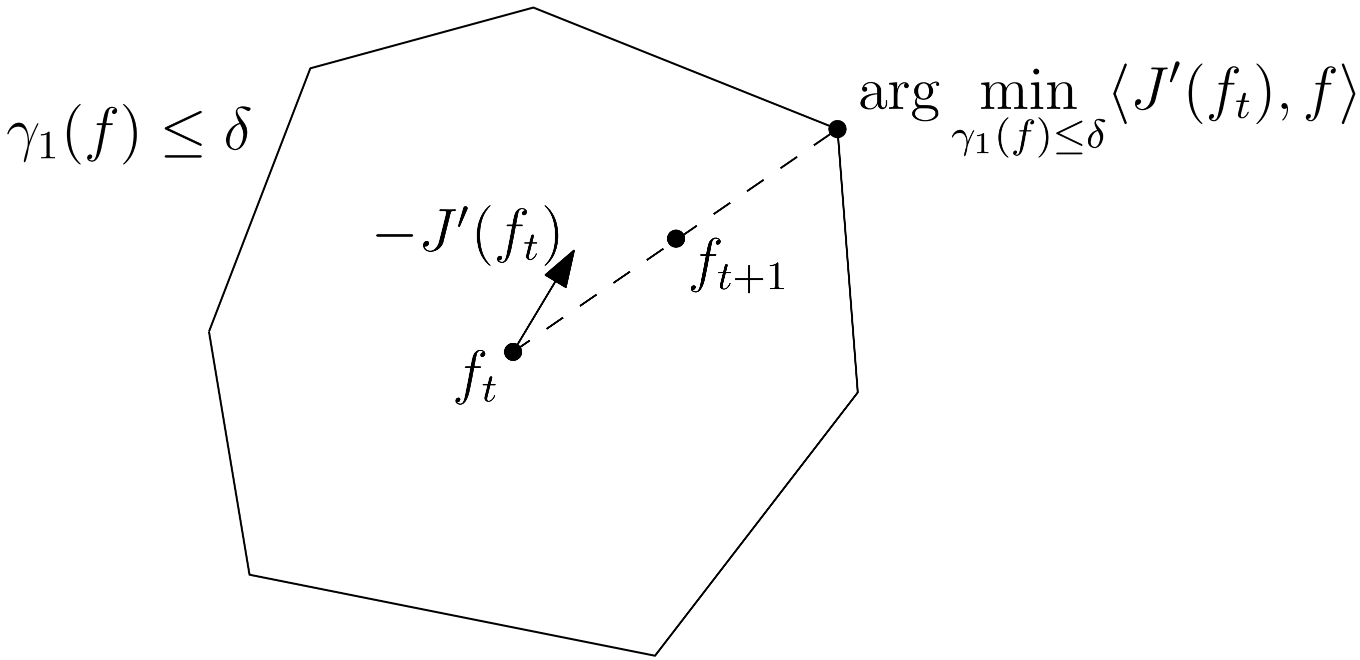
Variation norm and finite decomposition

- **Property 1** (Leshno et al., 1993): $\mathcal{F}_1$ is dense in L^2
- **Property 2** (Barron, 1993): for any $f \in \mathcal{F}_1$, there exists a finite decomposition $\hat{f}(x) = \sum_{i=1}^{k} \eta_i (w_i^\top x + b_i)_+$ such that
  - $\|f - \hat{f}\| \leqslant \varepsilon$ in L^2-norm
  - $k = O(\gamma_1(f)^2 \varepsilon^{-2})$
- NB: constructive proof by **conditional gradient algorithm**

Conditional gradient algorithm

- **Minimizing** $J(f)$ **such that** $\gamma_1(f) \leqslant \delta$
  - J smooth and convex
  - Frank-Wolfe, conditional gradient, gradient boosting, etc. (Frank and Wolfe, 1956; Dem'yanov and Rubinov, 1967; Dudik et al., 2012; Harchaoui et al., 2013; Jaggi, 2013)

- **Iteration**: $f_{t+1} = (1-\rho_t) f_t + \rho_t \operatorname*{argmin}_{\gamma_1(f) \leqslant \delta} \langle J'(f_t), f \rangle$



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  - Line search or $\rho_t = 2/(t+1)$
  - Convergence rate: $J(f) - \inf_{\gamma_1(g) \leqslant \delta} J(g) = O(\delta^2/t)$

- f_t **= convex combination of** t **extreme points**

Conditional gradient algorithm

Extreme points

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- f_t **= convex combination of t extreme points**
  - ℓ_1-ball: extreme points are 1-sparse vectors
  - The set $\{\gamma_1(f) \leqslant \delta\}$ is the convex hull of all functions

$$x \mapsto \pm\delta(w^\top x + b)_+, \text{ for } (w,b) \in \mathbb{R}^{d+1}$$

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- **Extreme points are single neurons/units**

$$\operatorname*{argmin}_{\gamma_1(f) \leqslant \delta} \langle J'(f_t), f \rangle = \pm\delta(w_t^\top \cdot + b_t)_+$$

  - for $(w_t, b_t) = -\operatorname{argmax}_{(w,b) \in \mathbb{R}^{d+1}} \big| \langle J'(f_t), (w^\top \cdot \; + b)_+ \rangle \big|$

Conditional gradient algorithm
Supervised learning from finite data set

- **Goal**: $\displaystyle \min_{\gamma_1(f)\leqslant\delta} \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i))$

- **Adding a new unit/neuron/basis function**:

$$\operatorname*{argmax}_{(w,b)\in\mathbb{R}^{d+1}} \left| \frac{1}{n}\sum_{i=1}^{n} g_i \cdot (w^\top x_i \ + b)_+ \right| \quad \text{with } g_i = \ell'(y_i, f_t(x_i))$$

  – Computational difficulty?

Adding extra neuron/unit for ReLUs

- Reformulation with $v = (w, b) \in \mathbb{R}^{d+1}$ and $z = (x, 1) \in \mathbb{R}^{d+1}$:

$$\max_{\|v\|_2 \leqslant 1} \left| \sum_{i=1}^{n} g_i (v^\top z_i)_+ \right| = \max_{\|v\|_2 \leqslant 1} \left| \sum_{i \in I_+} (v^\top t_i)_+ - \sum_{i \in I_-} (v^\top t_i)_+ \right|$$

with $I_+ = \{i, g_i \geqslant 0\}$ and $I_- = \{i, g_i < 0\}$, and $t_i = |g_i| z_i \in \mathbb{R}^{d+1}$,

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Hausdorff distance between zonotopes

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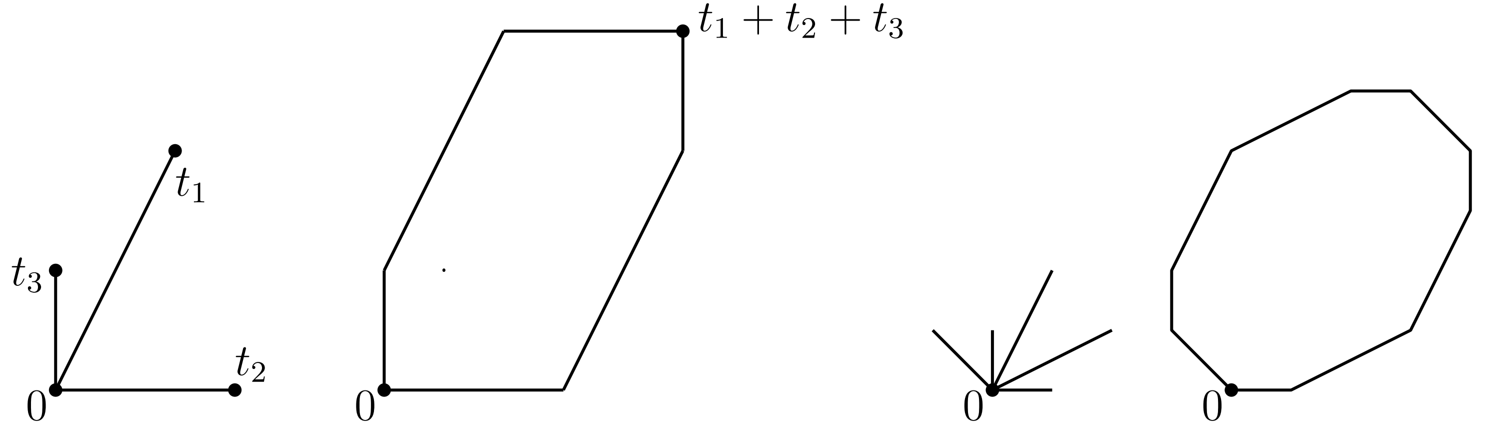
- By **convex duality**, equivalent to

$$\max \left\{ \min_{u_+ \in K_+} \max_{u_- \in K_-} \|u_+ - u_-\|_2, \min_{u_- \in K_-} \max_{u_+ \in K_+} \|u_+ - u_-\|_2 \right\}$$

with $K_+ = \left\{ \sum_{i \in I_+} b_i t_i, \; b_i \in [0, 1] \right\}$ and $K_- = \left\{ \sum_{i \in I_-} b_i t_i, \; b_i \in [0, 1] \right\}$

Hausdorff distance between zonotopes

- Zonotopes $K = \left\{ \sum_i b_i t_i,\ b_i \in [0,1] \right\}$ and zonoids (Bolker, 1969)



  - Affine projections of hypercubes
  - Zonoids are limits of zonotopes
  - In $d = 2$ (only), all centrally symmetric convex sets are zonoids

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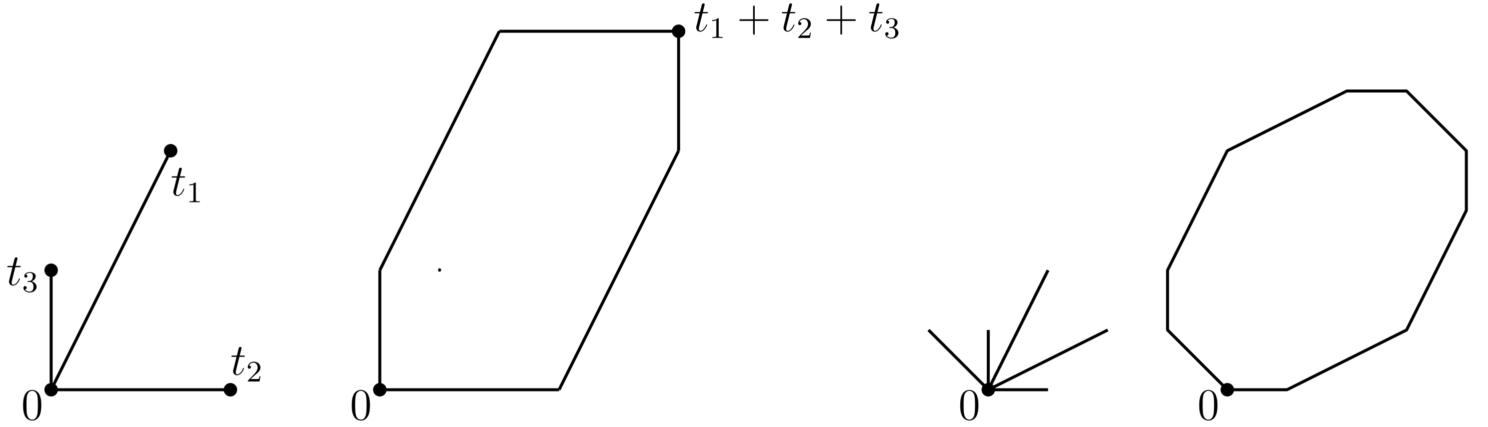
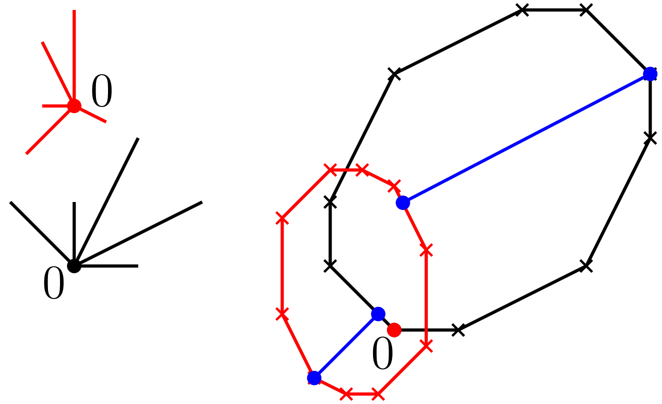


- **Hausdorff distance computation**, still hard...



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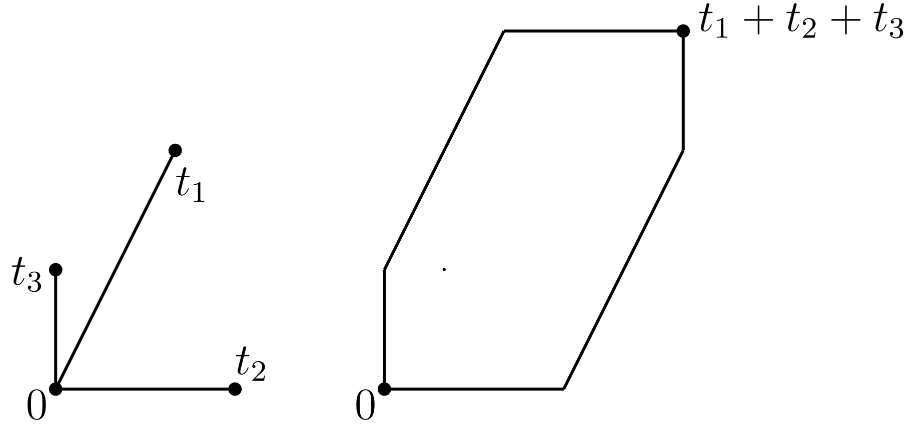
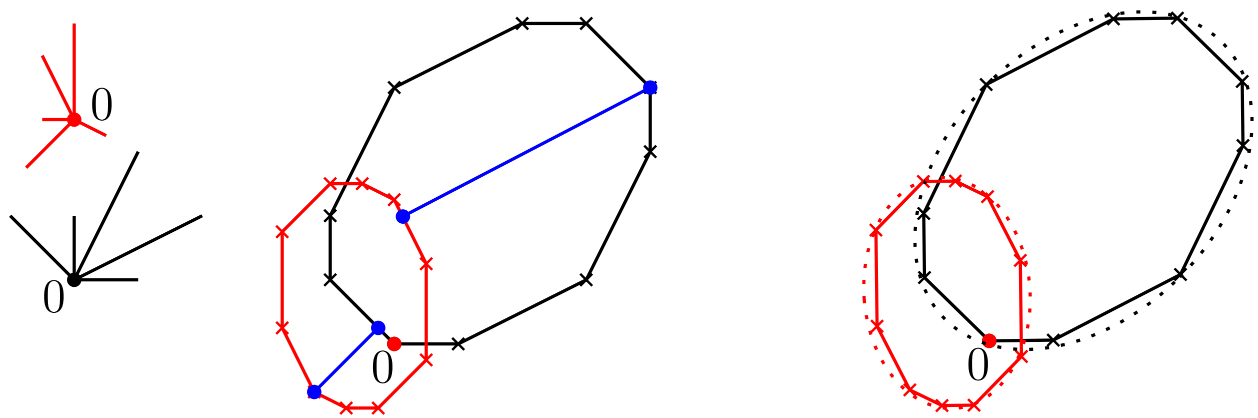


- **Hausdorff distance computation**, approximation by ellipsoids?



Convex relaxations and polynomial-time algorithms

- Many possibilities (SDP, ellipsoids, etc.), no success (yet)...

- (conjectured) **Impossible result**: for any $g \in \mathbb{R}^n$, find $\hat{v}$ such that $\|\hat{v}\|_2 = 1$ and

$$\Big| \sum_{i=1}^n g_i (\hat{v}^\top z_i)_+ \Big| \geqslant \frac{1}{\kappa} \max_{\|v\|_2=1} \Big| \sum_{i=1}^n g_i (v^\top z_i)_+ \Big|$$

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- **Sufficient result for matching generalization bounds**
  - Only in expectation for g standard Gaussian vector
  - Reduction to simple non-convex problem
  - NB: similar to linear binary classification (which is NP-hard)

Why not sampling weights?

- **Sampling** m weights (w_i, b_i) and use features $(w_i^\top x + b_i)_+$
  - Linear combination and ℓ_2-regularizer
  - Equivalent to a kernel $k(x,y) = \dfrac{1}{m}\sum_{i=1}^{m}(w_i^\top x + b_i)_+(w_i^\top y + b_i)_+$

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- **Letting** $m \to \infty$
  - $k(x,y)$ tends to $\displaystyle\int_{\mathbb{R}^{d+1}} (w^\top x + b)_+ (w^\top y + b)_+ d\mu(w,b)$
  - Random kernel expansion (Neal, 1995; Rahimi and Recht, 2007)
  - Can be computed in closed form (Le Roux and Bengio, 2007; Cho and Saul, 2009)

- Defines a **Hilbert space** $\mathcal{F}_2$ with norm γ_2 such that:

$$\gamma_2(f)^2 = \inf \int_{\mathbb{R}^{d+1}} |\eta(w,b)|^2 d\tau(w,b) \text{ s.t. } f(x) = \int_{\mathbb{R}^{d+1}} (w^\top x + b)_+ \eta(w,b) d\tau(w,b)$$

Generalization properties

- **Minimization of empirical risk** $\frac{1}{n}\sum_{i=1}^{n}\ell(y_i, f(x_i))$
  - subject to $\gamma_1(f) \leqslant \delta$: learning weights (w_j, b_j)
  - subject to $\gamma_2(f) \leqslant \delta$: sampling weights (w_j, b_j)
  - NB: $\gamma_1 \leqslant \gamma_2$, i.e., $\mathcal{F}_2 \subset \mathcal{F}_1$

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- **Sampling weights** (i.e., using ℓ_2 / kernel methods)
  - No adaptivity (e.g., a single neuron does not belong to $\mathcal{F}_2$)

- **Learning sparse weights** (i.e., using ℓ_1)
  - Automatic adaptivity to structure
  - E.g., $f(x) = g(W^\top x)$ for W of low-rank

Approximation properties with variation norm

- **Finite variation norm**
  - f $(d/2+3/2)$-times differentiable $\Rightarrow \gamma_1(f) \leqslant \gamma_2(f) < \infty$
  - Smoothness index has to grow with dimension!

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- **Approximation of Lipschitz-continuous functions**
  - f 1-Lipschitz-continuous $\Rightarrow$ there exists g such that $\gamma_1(g) \leqslant \delta$ and with approximation error $\delta^{-2/(d+1)} \log \delta$
  - Proof based on spherical harmonics

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- **Adaptivity**
  - If f depends on a s-dimensional projection, replace d by s
  - Only works for γ_1

Generalization bounds

- Assuming f^* of a certain form
  - Penalizing weight vectors w by ℓ_2-norms

function space	$\|\cdot\|_2$
$w^\top x + b$	$\frac{d^{1/2}}{n^{1/2}}$
No assumption	$\frac{C(d)}{n^{1/(d+3)}} \log n$
$\sum_{j=1}^{k} f_j(w_j^\top x),\ w_j \in \mathbb{R}^d$	$\frac{kd^{1/2}}{n^{1/4}} \log n$
$\sum_{j=1}^{k} f_j(W_j^\top x),\ W_j \in \mathbb{R}^{d \times s}$	$\frac{kd^{1/2}C(s)}{n^{1/(s+3)}} \log n$

Generalization bounds

- Assuming f^* of a certain form
  - Penalizing weight vectors w by ℓ_2-norms
  - Assuming q-sparse solution and penalizing w by ℓ_1-norm

function space	$\|\cdot\|_2$	$\|\cdot\|_1$
$w^\top x + b$	$\frac{d^{1/2}}{n^{1/2}}$	$\sqrt{q}\frac{(\log d)^{1/2}}{n^{1/2}}$
No assumption	$\frac{C(d)}{n^{1/(d+3)}} \log n$	$\frac{q^{1/2}C(d)}{n^{1/(d+3)}} \log n$
$\sum_{j=1}^{k} f_j(w_j^\top x),\ w_j \in \mathbb{R}^d$	$\frac{kd^{1/2}}{n^{1/4}} \log n$	$\frac{kq^{1/2}(\log d)^{1/2}}{n^{1/4}} \log n$
$\sum_{j=1}^{k} f_j(W_j^\top x),\ W_j \in \mathbb{R}^{d\times s}$	$\frac{kd^{1/2}C(s)}{n^{1/(s+3)}} \log n$	$\frac{kq^{1/2}C(s)(\log d)^{2/(s+3)}}{n^{1/(s+3)}} \log n$

Conclusion

- **Convex neural networks / infinitely many basis functions**
  - Adaptivity to structure
  - Corresponding ernel methods are not adaptive
  - Provable high-dimensional non-linear variable selection
- **Convex but no polynomial-time algorithm**
  - Reduction to approximate Haussdorff distance between zonotopes
  - Open problem

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- **Extensions**
  - Multiple outputs
  - Multiple layers
  - Other models (e.g., Gaussian mixtures)

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