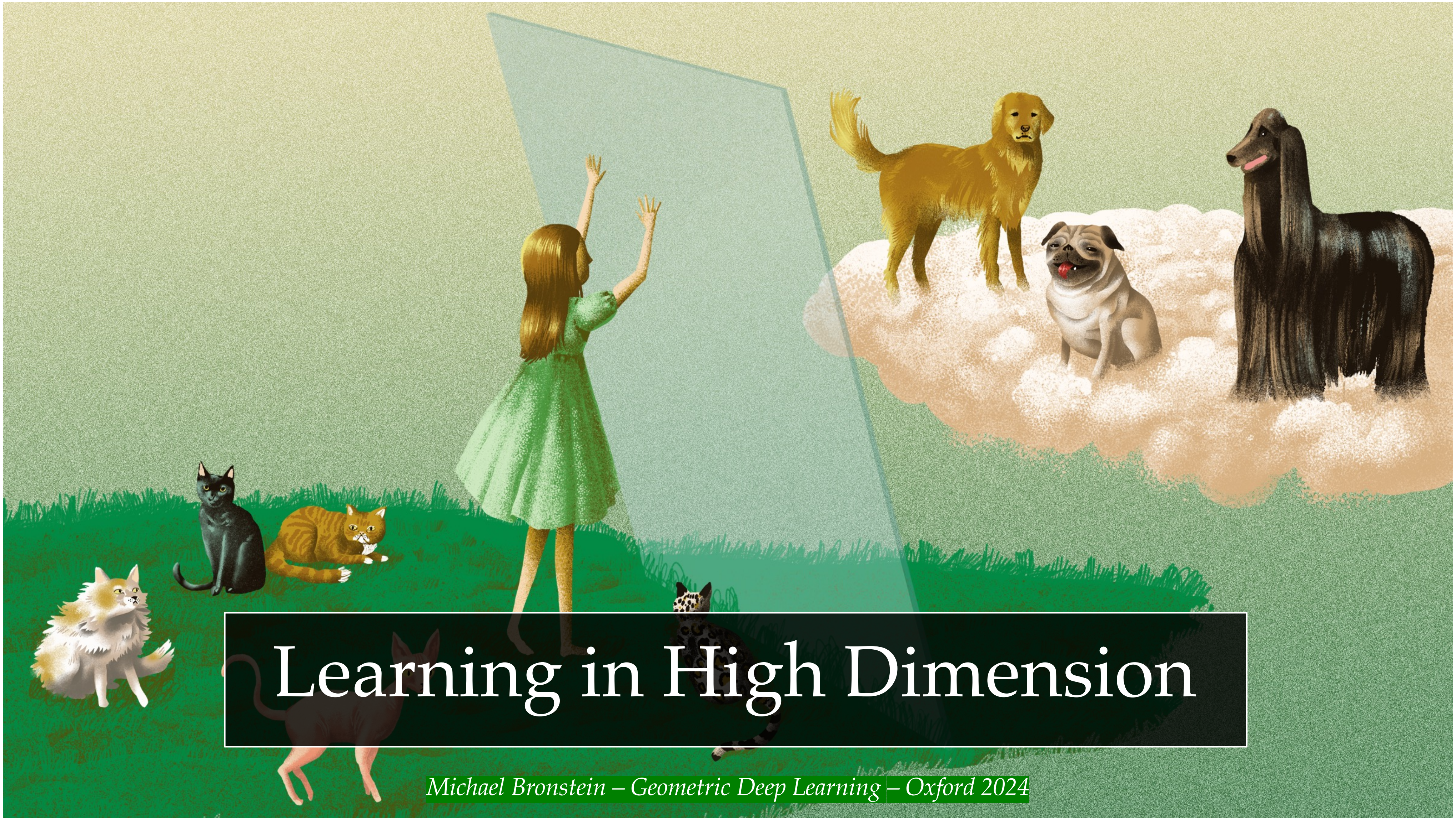


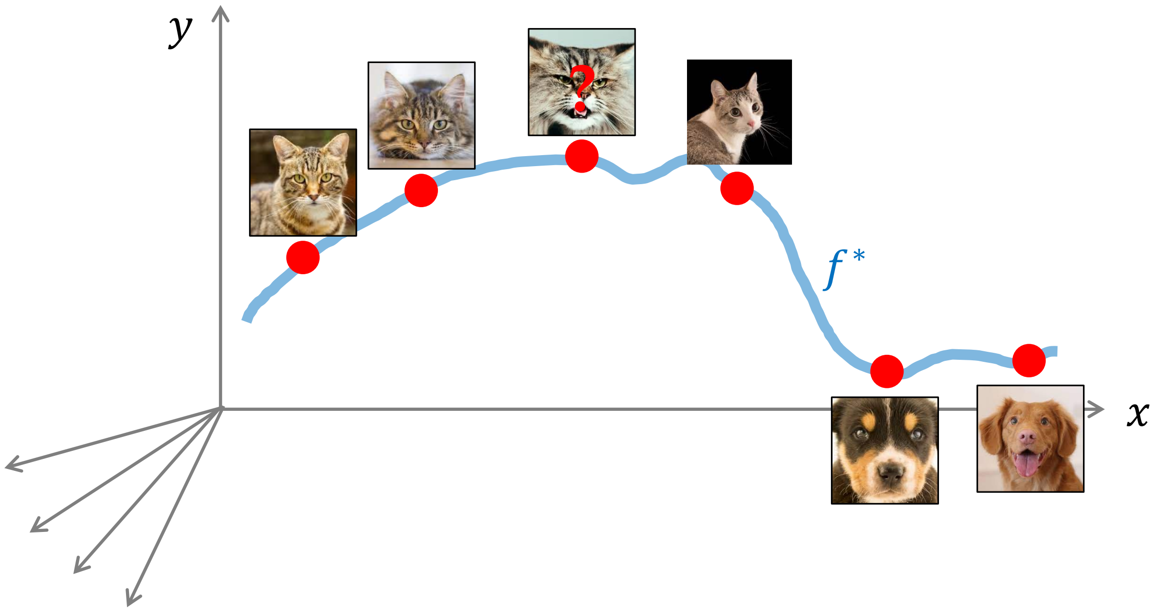
Learning in High Dimension
Michael Bronstein – Geometric Deep Learning – Oxford 2024

Outline

- Supervised machine learning has three sources of error: *approximation*, *estimation*, and *optimisation*
- Dealing with high-dimensional inputs requires strong notions of *regularity*
- Standard function classes based on local/global continuity are *dimensionality-cursed*
- This will bring us to the need for a new *geometric* type of regularity, which is at the core of Geometric Deep Learning

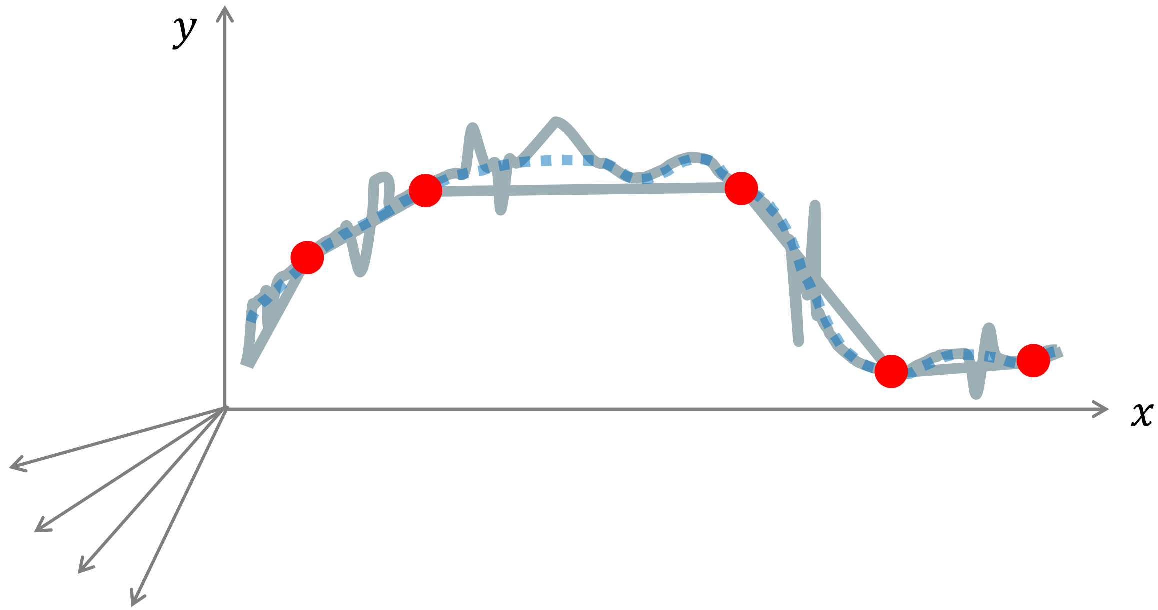

ML
black
box
{cat,dog}

(Supervised) Machine Learning = glorified curve fitting



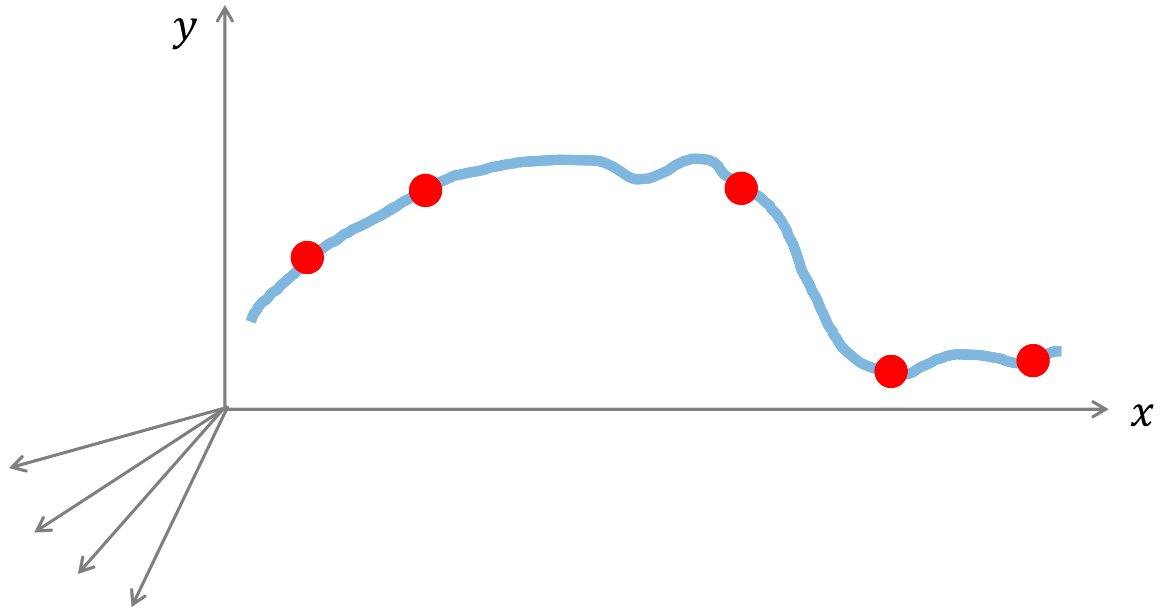
Given a set of observations $\{(x_i, y_i)\}_{i=1}^N$ of some function f^* ("*training set*") predict its values at previously unseen points

(Supervised) Machine Learning = glorified curve fitting



How the function looks like?

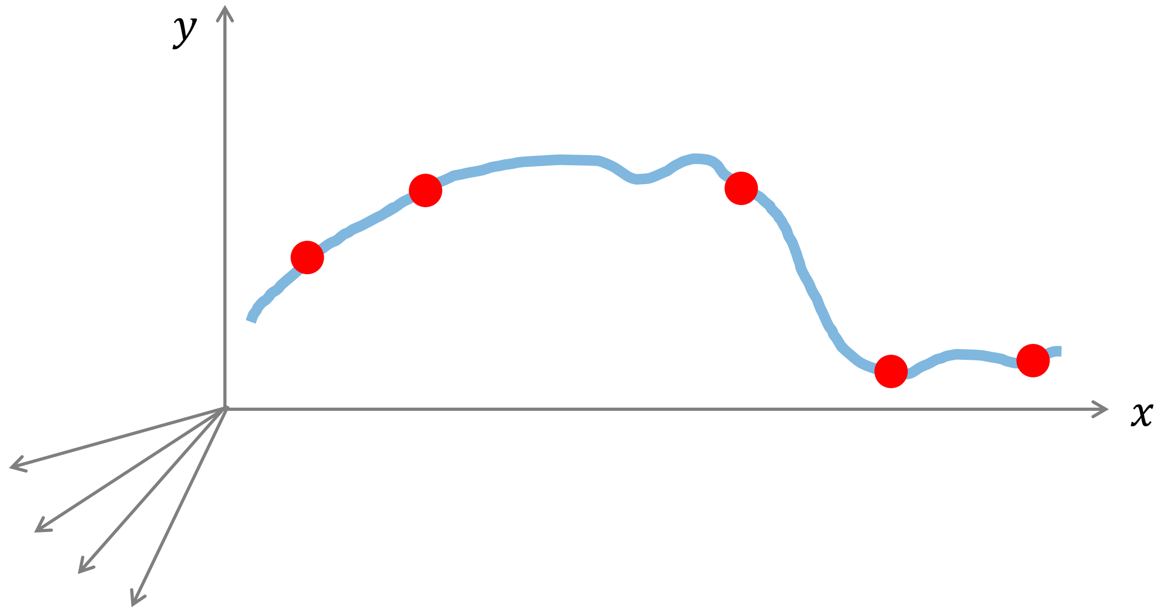
(Supervised) Machine Learning = glorified curve fitting



How the function looks like?

How the sampling looks like?

(Supervised) Machine Learning = glorified curve fitting



How the function looks like?

approximation

How the sampling looks like?

estimation

How to find the fitting?

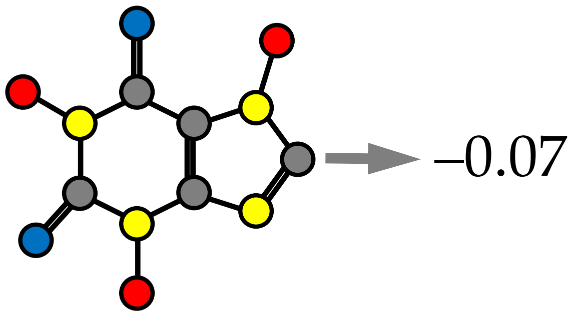
optimisation

BASICS OF STATISTICAL MACHINE LEARNING

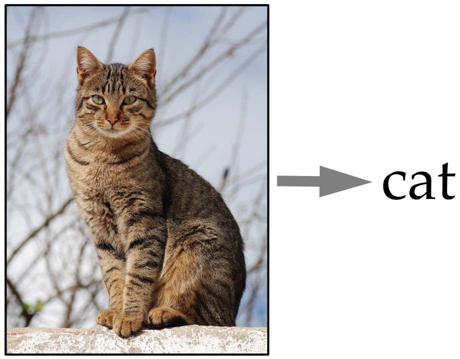
Problem setting

- **Inputs** $x_i \in \mathcal{X}$ typically high dimensional (e.g. $\mathcal{X} = \mathbb{R}^d$, $d \gg 1$)
- **Labels** $y_i \in \mathcal{Y}$
  - *Regression:* $\mathcal{Y} = \mathbb{R}$
  - *Classification:* $\mathcal{Y} = \{1, \ldots, K\}$
  - *Structured prediction:* $\mathcal{Y} = \mathcal{X}$

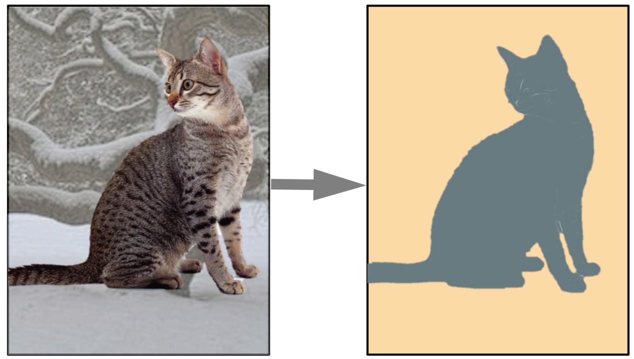
Examples of Supervised Learning problems



Regression
(solubility log$P$)



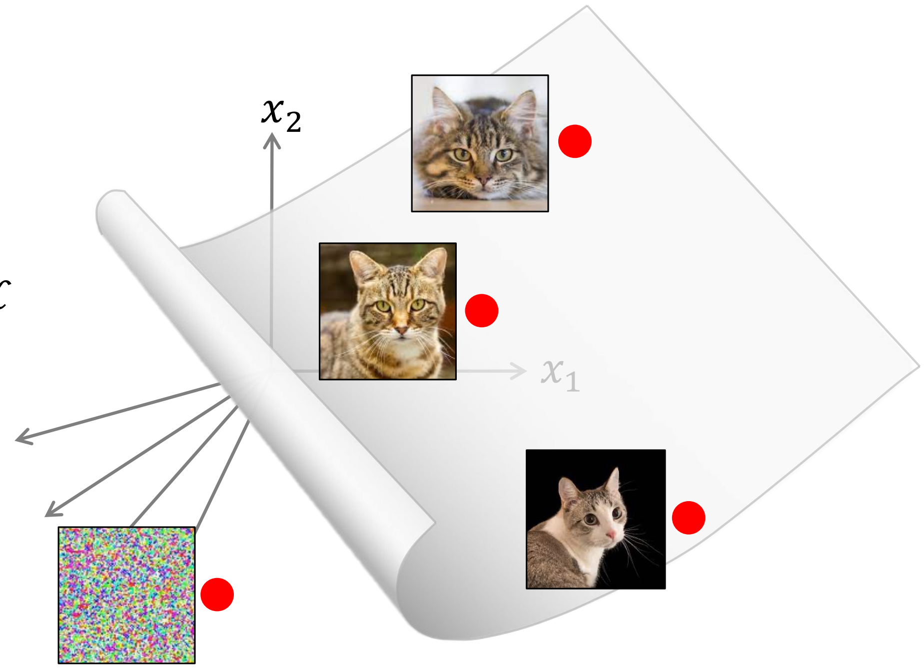
Classification
(binary: cat/dog)



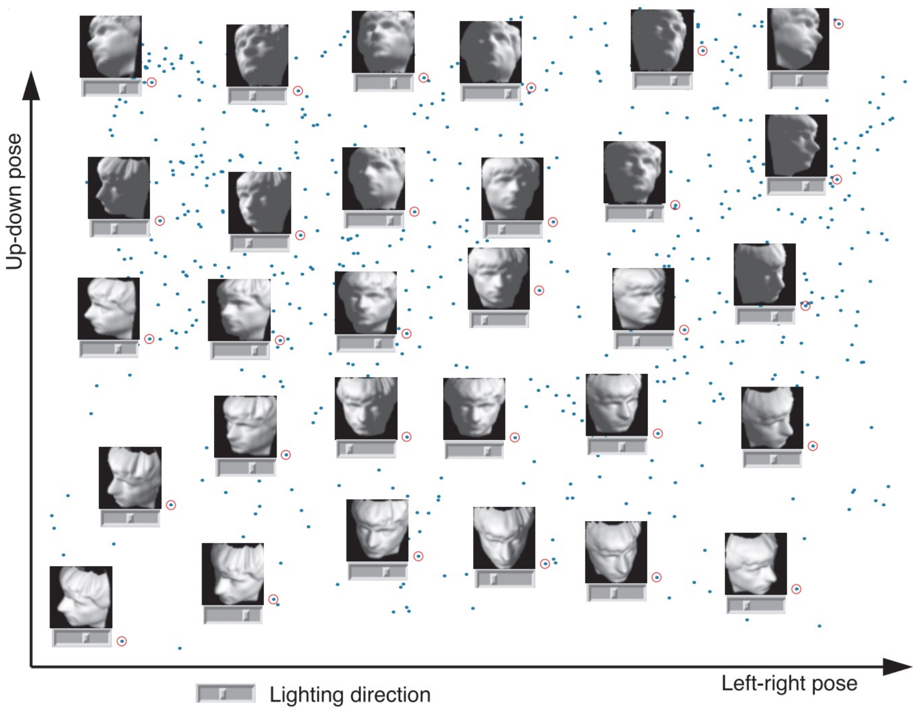
Structured prediction
(image segmentation)

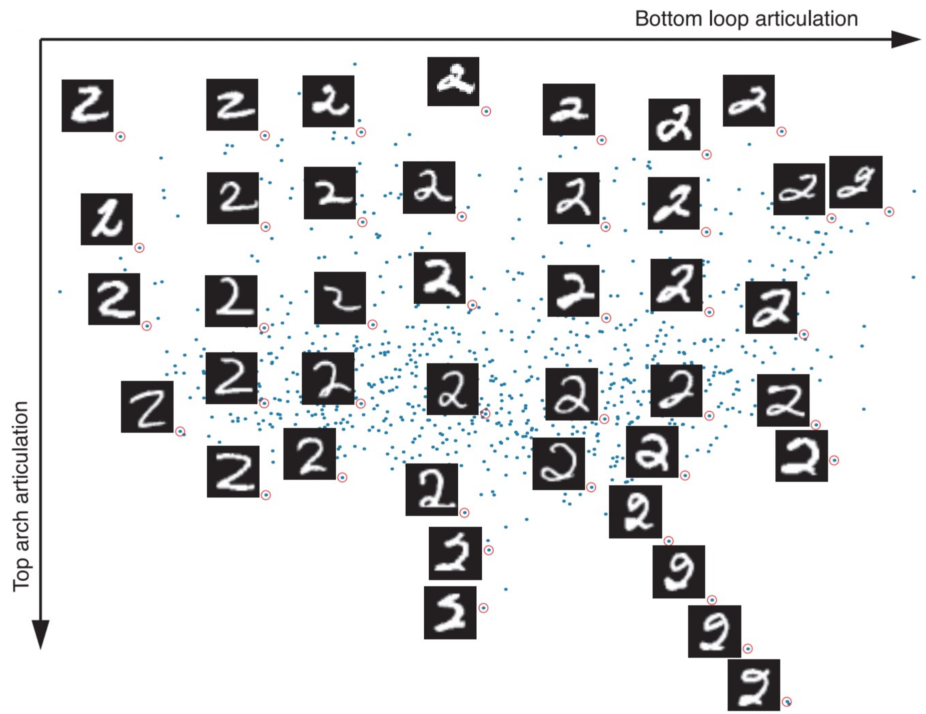
Data

- **Data distribution** $P(x, y)$
  - Distribution P is *unknown* during learning
  - Samples assumed to be drawn *i.i.d.*
  - Often forms a low-dimensional structure in $\mathcal{X}$ (*“manifold assumption”*)



Manifold Assumption





Tenenbaum, De Silva, Langford 2000

Error metric

- **Loss function** $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ satisfying $\ell(y, y') \geq 0$ and $\ell(y, y) = 0$
  - *Classification loss:* $\ell(y, y') \geq 1_{y \neq y'}$
  - *Regression loss:* $\ell(y, y') = \|y - y'\|^2$
- Given a function $f: \mathcal{X} \to \mathcal{Y}$, the loss $\ell(f(x), y)$ is a *random variable*

Error metric

- **Loss function** $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ satisfying $\ell(y, y') \geq 0$ and $\ell(y, y) = 0$
- **Population risk** (or **error**) of f

$$\mathcal{R}(f) = \mathbb{E}\ell(f(x), y) = \int_{\mathcal{X}\times\mathcal{Y}} \ell(f(x), y)\mathrm{d}P(x, y)$$

$$= \mathbb{E}_x \ \mathbb{E}_{y|x}[\ell(f(x), y)|x] = \int_{\mathcal{X}} \int_{\mathcal{Y}} \ell(f(x), y)\mathrm{d}P_{y|x}(y) \ \mathrm{d}P_x(x)$$

Conditioning on x

Error metric

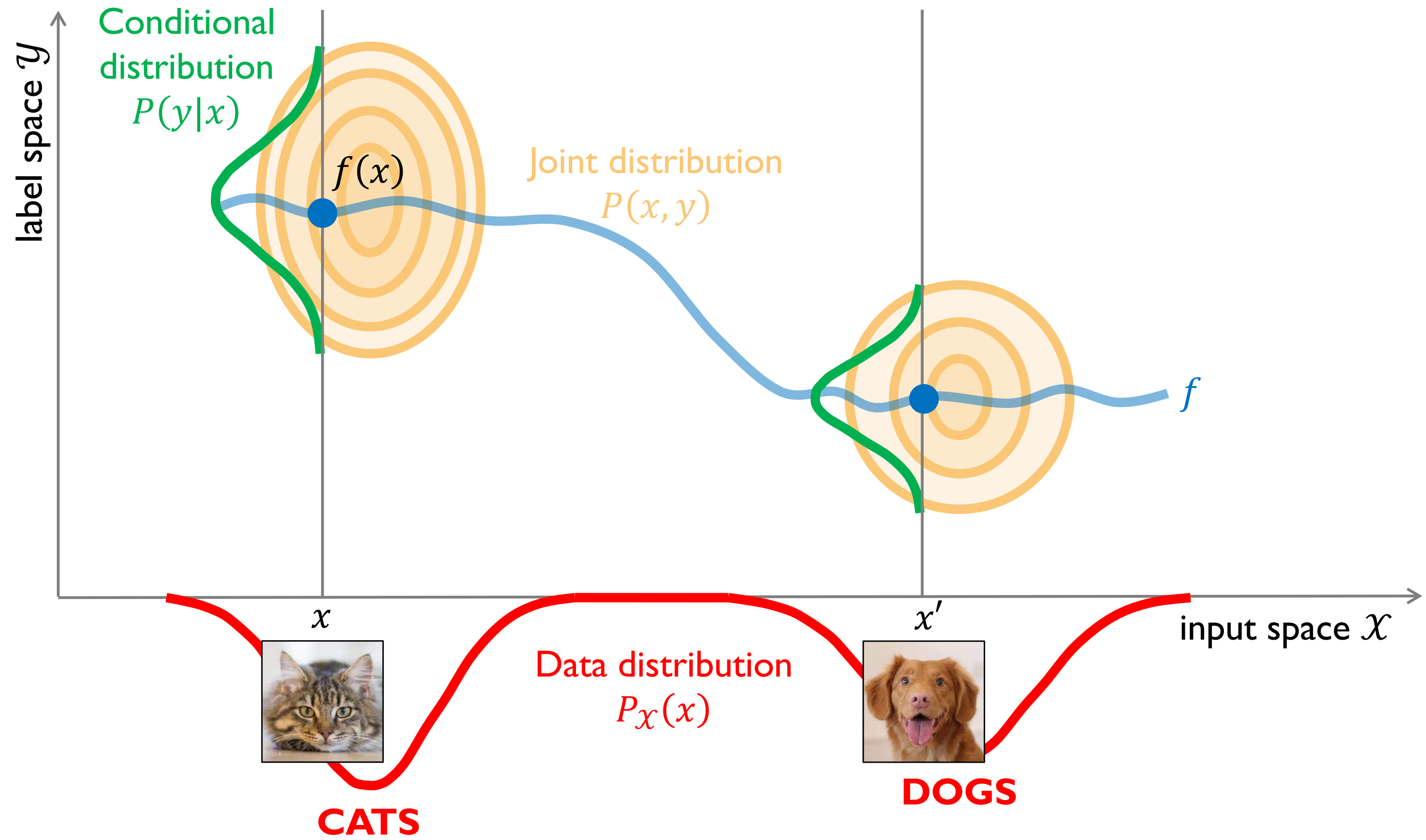
- **Loss function** $\ell\colon \mathcal{Y}\times\mathcal{Y} \to \mathbb{R}$ satisfying $\ell(y, y') \geq 0$ and $\ell(y, y) = 0$
- **Population risk** (or **error**) of f

$$\mathcal{R}(f) = \mathbb{E}\ell(f(x), y) = \mathbb{E}_x \mathbb{E}_{y|x}[\ell(f(x), y)|x]$$

- **Bayes optimal estimator** minimises the error *point-wise*

$$f^*(x) = \operatorname*{argmin}_{z\in\mathcal{Y}} \mathbb{E}_{y|x}[\ell(z, y)|x]$$

  - Defined via distribution P, which is *unknown in practice*
  - f^* may be *arbitrarily complex*



Conditional
distribution
$P(y|x)$
label space $\mathcal{Y}$
$f(x)$
Joint distribution
$P(x, y)$
f
x
x'
input space $\mathcal{X}$
Data distribution
$P_{\mathcal{X}}(x)$
CATS
DOGS

Model class

- **Hypothesis** (or **model**) **class** is a subset of functions $\mathcal{F} = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta\}$
  - *Polynomials of degree k*: $f_\theta(x) = \sum_{i=0}^{k} \theta_i x^i$
  - *Neural networks* of certain type (with θ being layer weights)

Model class

- **Hypothesis** (or **model**) **class** is a subset of functions $\mathcal{F} = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta\}$
- **Model complexity** (or **capacity**) is some non-negative function $\gamma : \Theta \to \mathbb{R}$ allowing to order the functions in $\mathcal{F}$ according to their "complexity"
  - *Weight decay* $\gamma(\theta) = \|\theta\|_p^p$ in a linear model $f_\theta(x) = \langle \theta, x \rangle$
  - *Number of neurons* in a neural network
  - *Sobolev norm* $\gamma(\theta) = \int_{\mathbb{R}} (1 + \omega^2)^s \left|\hat{f}_\theta(\omega)\right|^2 \mathrm{d}\omega$

Sobolev space $H^s = W^{s,2}$ is a generalization of the Lebesgue space L_2 (square-integrable functions) accounting for the function's derivatives

Note: confusingly, $\hat{f}$ here denotes the Fourier transform of f

Model class

- **Hypothesis** (or **model**) **class** is a subset of functions $\mathcal{F} = \{f_\theta : \mathcal{X} \to \mathcal{Y} \,:\, \theta \in \Theta\}$
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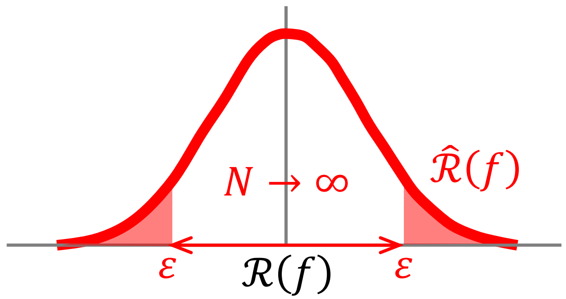
  - *Sobolev norm* $\gamma(\theta) = \int_{\mathbb{R}} (1 + \omega^2)^s \left|\hat{f}_\theta(\omega)\right|^2 \mathrm{d}\omega$
  - *Implicitly defined* through optimisation algorithm (e.g. gradient descent of under-determined least-squares problem converges to interpolating solution with minimum L_2-norm)

Empirical risk

- **Empirical risk** (or **error**) replaces the expectation of the loss with an average on the training set $\{(x_i, y_i)\}_{i=1}^N$:

$$\hat{\mathcal{R}}(f) = \frac{1}{N}\sum_{i=1}^{N} \ell(f(x_i), y_i)$$

  - *Generalisation gap* $= \hat{\mathcal{R}}(f) - \mathcal{R}(f)$
  - $\hat{\mathcal{R}}(f)$ is a random function serving an *unbiased estimator* of $\mathcal{R}(f)$
  - *Variance* $\sigma(f) \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$
  - *Hoeffding inequality* $P\left(\left|\hat{\mathcal{R}}(f) - \mathcal{R}(f)\right| > \varepsilon\right) \leq 2e^{-2\varepsilon^2 N}$
    "$\hat{\mathcal{R}}(f) = \mathcal{R}(f)$ is **probably approximately correct**"
  - Tells how good a given f is but not the model class $\mathcal{F}$
    (more delicate analysis: *VC dimension*, *Rademacher complexity*)



Empirical risk minimisation

- Supervised learning = minimisation of the **empirical risk** over a training set $\{(x_i, y_i)\}_{i=1}^{N}$ w.r.t. the parameters of a model class $\mathcal{F} = \{f_\theta : \mathcal{X} \rightarrow \mathcal{Y} \,:\, \theta \in \Theta\}$:

$$\hat{\theta} \in \operatorname*{argmin}_{\theta \in \Theta} \hat{\mathcal{R}}(f_\theta)$$

  in hope that the estimator $\hat{f} = f_{\hat{\theta}}$ generalises well, i.e., **excess risk** $\mathcal{R}(\hat{f}) - \mathcal{R}(f^*)$ is small

  - Usually a non-convex problem, can be solved only approximately!
  - Achieving a small **training error** $\hat{\mathcal{R}}(f_{\hat{\theta}})$ fundamentally depends on the richness of the model class (often, number of parameters $|\Theta|$)
  - Deep learning typically operates in *overparametrised regime* ($|\Theta| \gg N$), where multiple solutions are possible
  - How to make an informed choice among these solutions?

Regularisation

- **Regularisation** (or **capacity control**): find the "simplest" solution by restricting the model capacity *("Occam's razor principle"*)
  - *Constrained form:* $\hat{\theta}_\delta = \operatorname*{argmin}_{\theta\in\Theta} \hat{\mathcal{R}}(f_\theta) \quad \text{s.t.} \quad \gamma(\theta) \leq \delta$
  - *Penalised form:* $\hat{\theta} = \operatorname*{argmin}_{\theta\in\Theta} \hat{\mathcal{R}}(f_\theta) \ + \ \lambda\gamma(\theta)$
  - *Interpolation form:* $\hat{\theta} = \operatorname*{argmin}_{\theta\in\Theta} \gamma(\theta) \quad \text{s.t.} \quad \hat{\mathcal{R}}(f_\theta) = 0$
  - *Implicit form:* stems from the optimisation algorithm

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\widehat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} \, : \, \theta \in \Theta, \ \gamma(\theta) \leq \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*)$$

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \le \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) = \mathcal{R}(\hat{f}) - \boxed{\min_{\gamma(\theta)\le\delta} \mathcal{R}(f_\theta)} + \min_{\gamma(\theta)\le\delta} \mathcal{R}(f_\theta) - \mathcal{R}(f^*)$$

best model

$f_{\theta^*} \in \mathcal{F}_\delta$

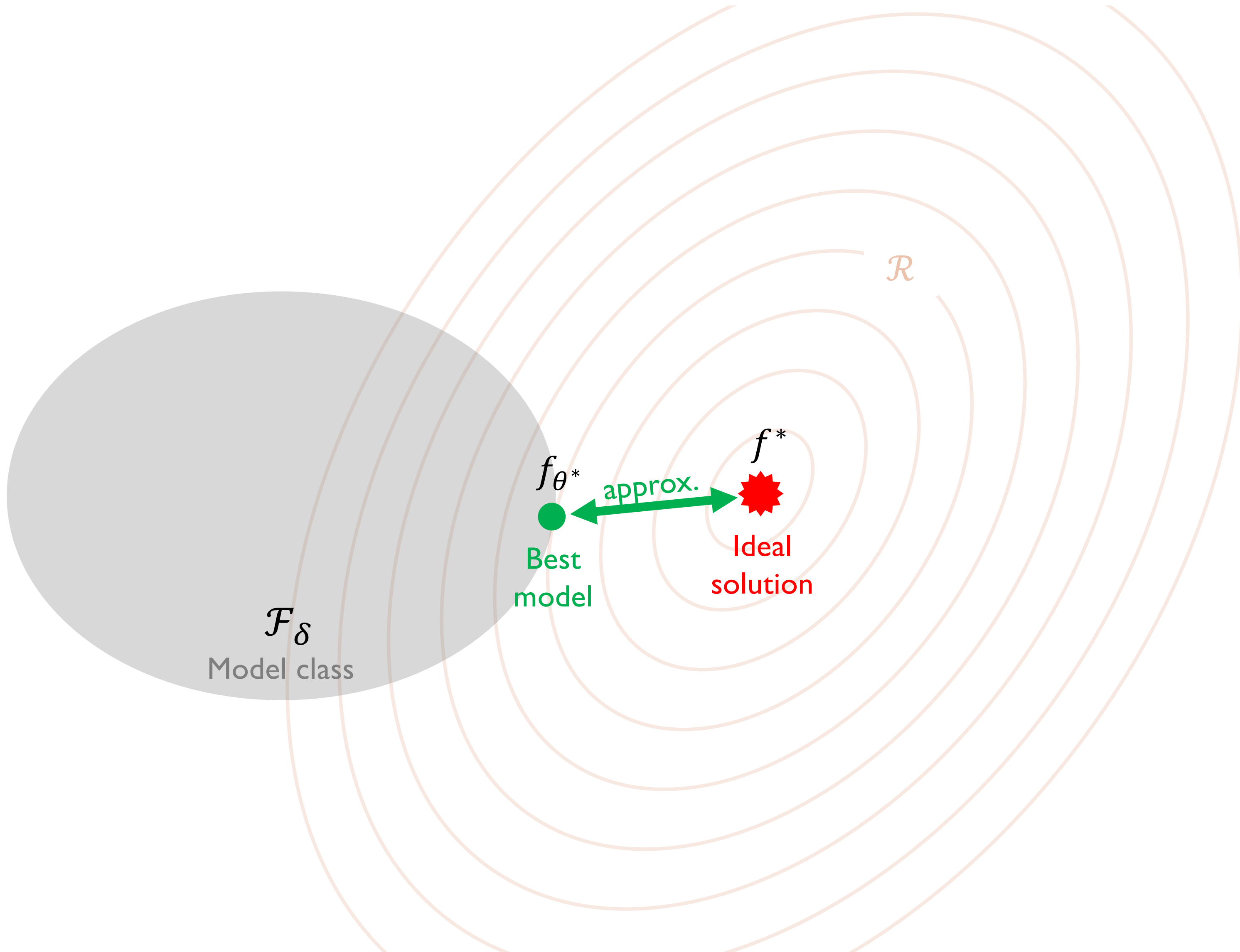
Note: Here we assume for simplicity the min is attained (more generally, should be inf)

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \leq \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) = \mathcal{R}(\hat{f}) - \mathcal{R}(f_{\theta^*}) + \boxed{\mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)}$$

approximation error
"how expressive $\mathcal{F}_\delta$ is"



$\mathcal{R}$
f^*
f_{θ^*}
approx.
Best
model
Ideal
solution
$\mathcal{F}_\delta$
Model class

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \le \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) = \mathcal{R}(\hat{f}) - \mathcal{R}(f_{\theta^*}) + \mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)$$

approximation error
"how expressive $\mathcal{F}_\delta$ is"

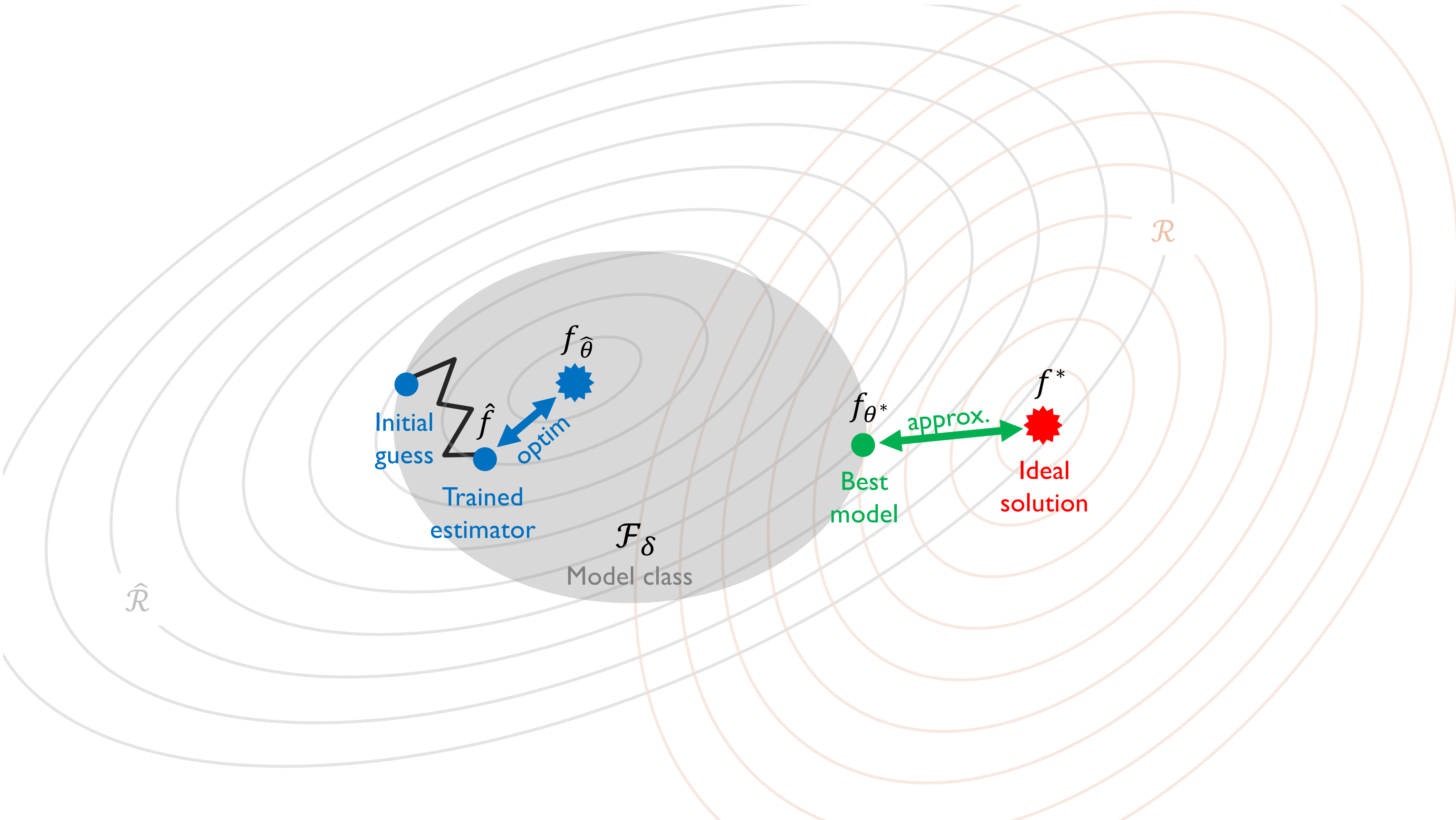
Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \leq \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) = \mathcal{R}(\hat{f}) - \hat{\mathcal{R}}(\hat{f}) + \hat{\mathcal{R}}(f_{\hat{\theta}}) - \mathcal{R}(f_{\theta^*}) + \underbrace{\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(f_{\hat{\theta}})}_{\text{optimisation error}} + \underbrace{\mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)}_{\text{approximation error}}$$

optimisation error
"how far $\hat{f}$ is from $f_{\hat{\theta}}$"

approximation error
"how expressive $\mathcal{F}_\delta$ is"



$\mathcal{R}$
$f_{\hat{\theta}}$
f^*
f_{θ^*}
approx.
Initial
guess
$\hat{f}$
optim
Trained
estimator
Best
model
Ideal
solution
$\mathcal{F}_\delta$
Model class
$\hat{\mathcal{R}}$

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \le \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) = \mathcal{R}(\hat{f}) - \hat{\mathcal{R}}(\hat{f}) + \boxed{\hat{\mathcal{R}}(f_{\hat{\theta}}) - \mathcal{R}(f_{\theta^*})} + \boxed{\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(f_{\hat{\theta}})} + \boxed{\mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)}$$

$$\hat{\mathcal{R}}(f_{\hat{\theta}}) = \min_{\gamma(\theta) \le \delta} \hat{\mathcal{R}}(f) \le \hat{\mathcal{R}}(f_{\theta^*})$$

optimisation error
"how far $\hat{f}$ is from $f_{\hat{\theta}}$"

approximation error
"how expressive $\mathcal{F}_\delta$ is"

Error decomposition

- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \leq \delta\}$

$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) \leq \mathcal{R}(\hat{f}) - \hat{\mathcal{R}}(\hat{f}) + \hat{\mathcal{R}}(f_{\theta^*}) - \mathcal{R}(f_{\theta^*}) + \hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(f_{\hat{\theta}}) + \mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)$$

optimisation error
"how far $\hat{f}$ is from $f_{\hat{\theta}}$"

approximation error
"how expressive $\mathcal{F}_\delta$ is"

Error decomposition

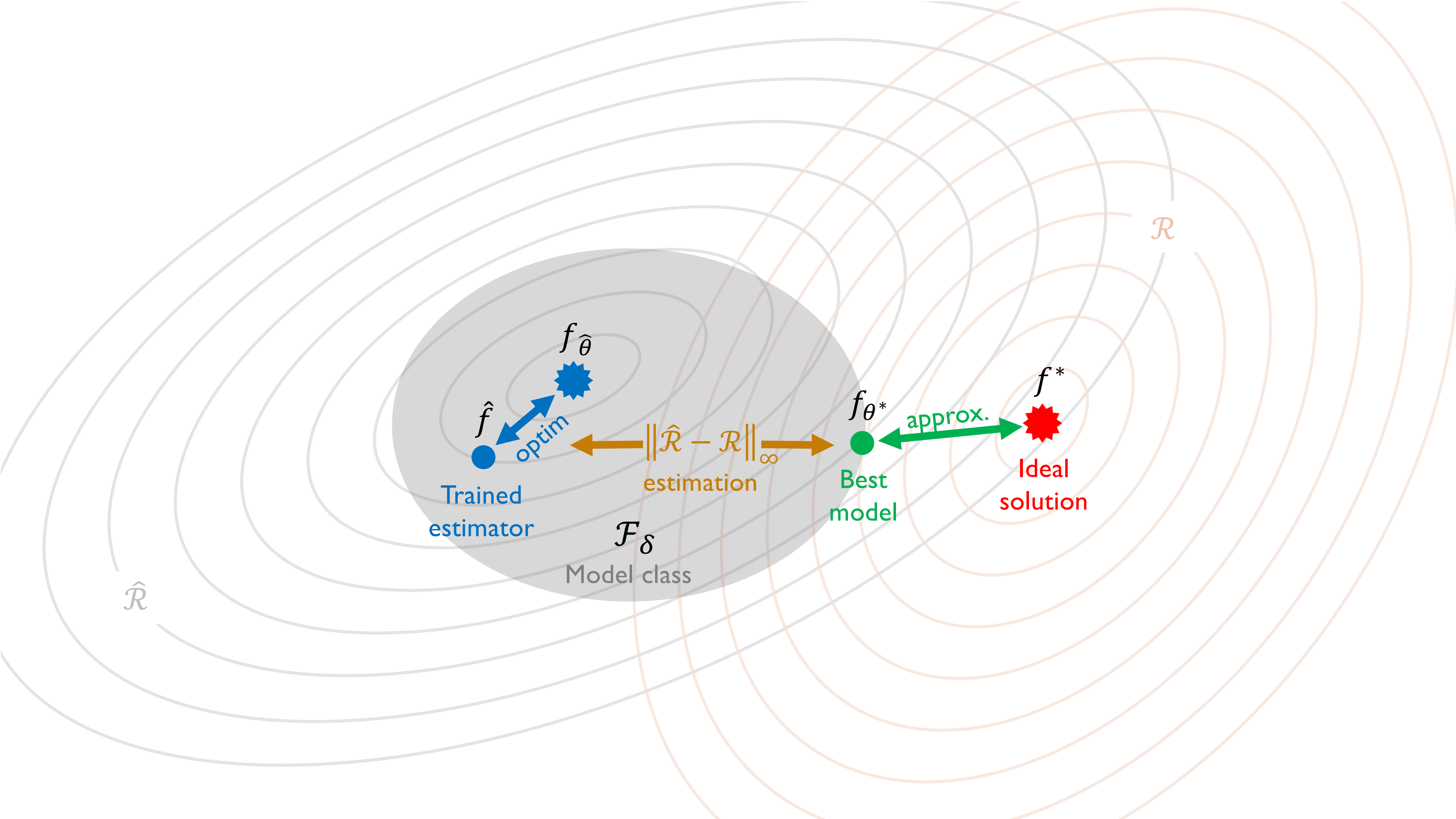
- **Excess risk** of the estimator $\hat{f} \approx f_{\hat{\theta}}$ obtained by (approximate) constrained empirical risk minimisation over a nested family of functions $\mathcal{F}_\delta = \{f_\theta : \mathcal{X} \to \mathcal{Y} : \theta \in \Theta,\ \gamma(\theta) \leq \delta\}$

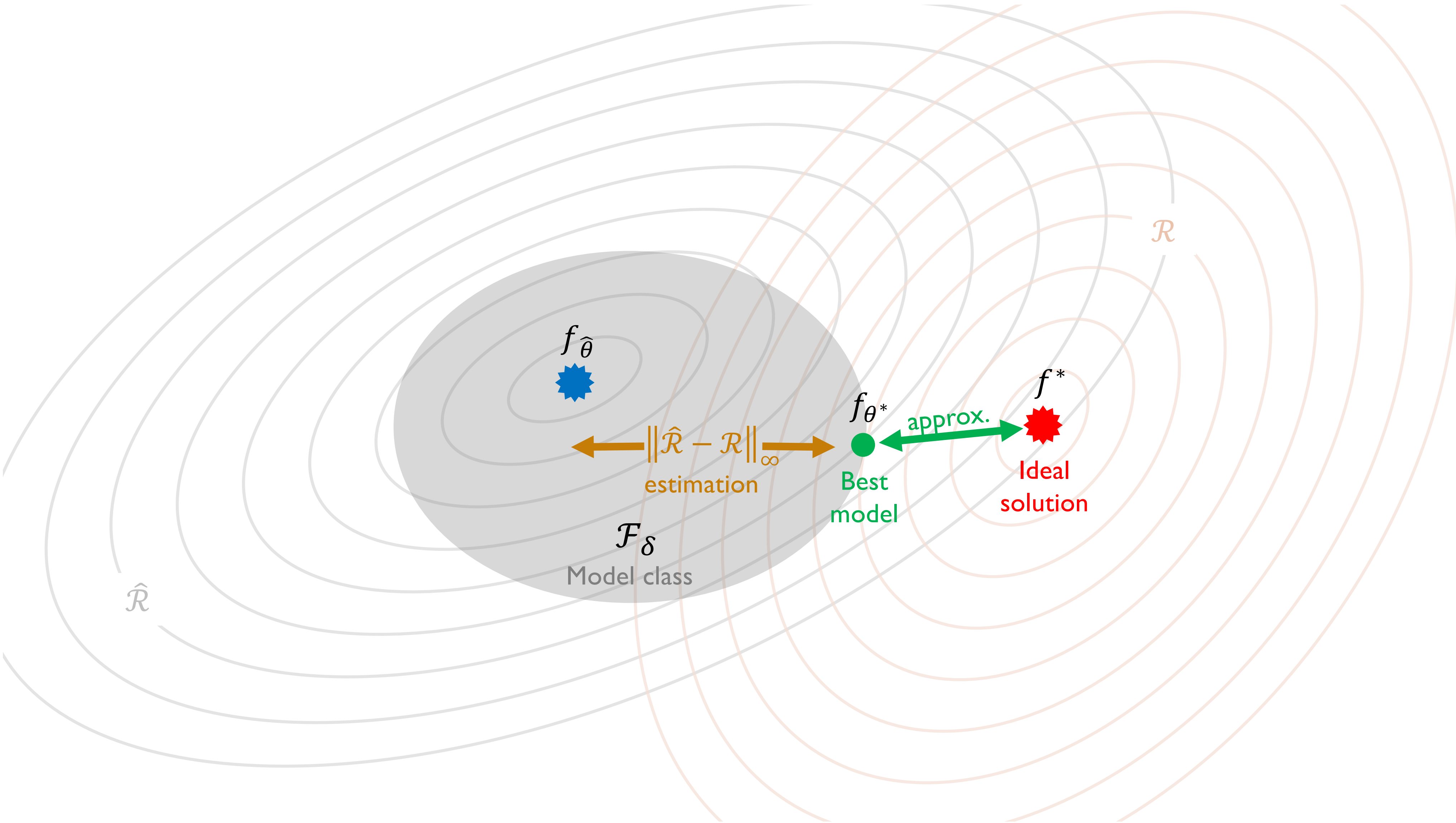
$$\mathcal{R}(\hat{f}) - \mathcal{R}(f^*) \leq \underbrace{2 \sup_{\gamma(\theta)\leq\delta} \left|\hat{\mathcal{R}}(f_\theta) - \mathcal{R}(f_\theta)\right|}_{\text{estimation error}} + \underbrace{\hat{\mathcal{R}}(\hat{f}) - \hat{\mathcal{R}}(f_{\hat{\theta}})}_{\text{optimisation error}} + \underbrace{\mathcal{R}(f_{\theta^*}) - \mathcal{R}(f^*)}_{\text{approximation error}}$$

estimation error
"how far the empirical risk is from the population risk"

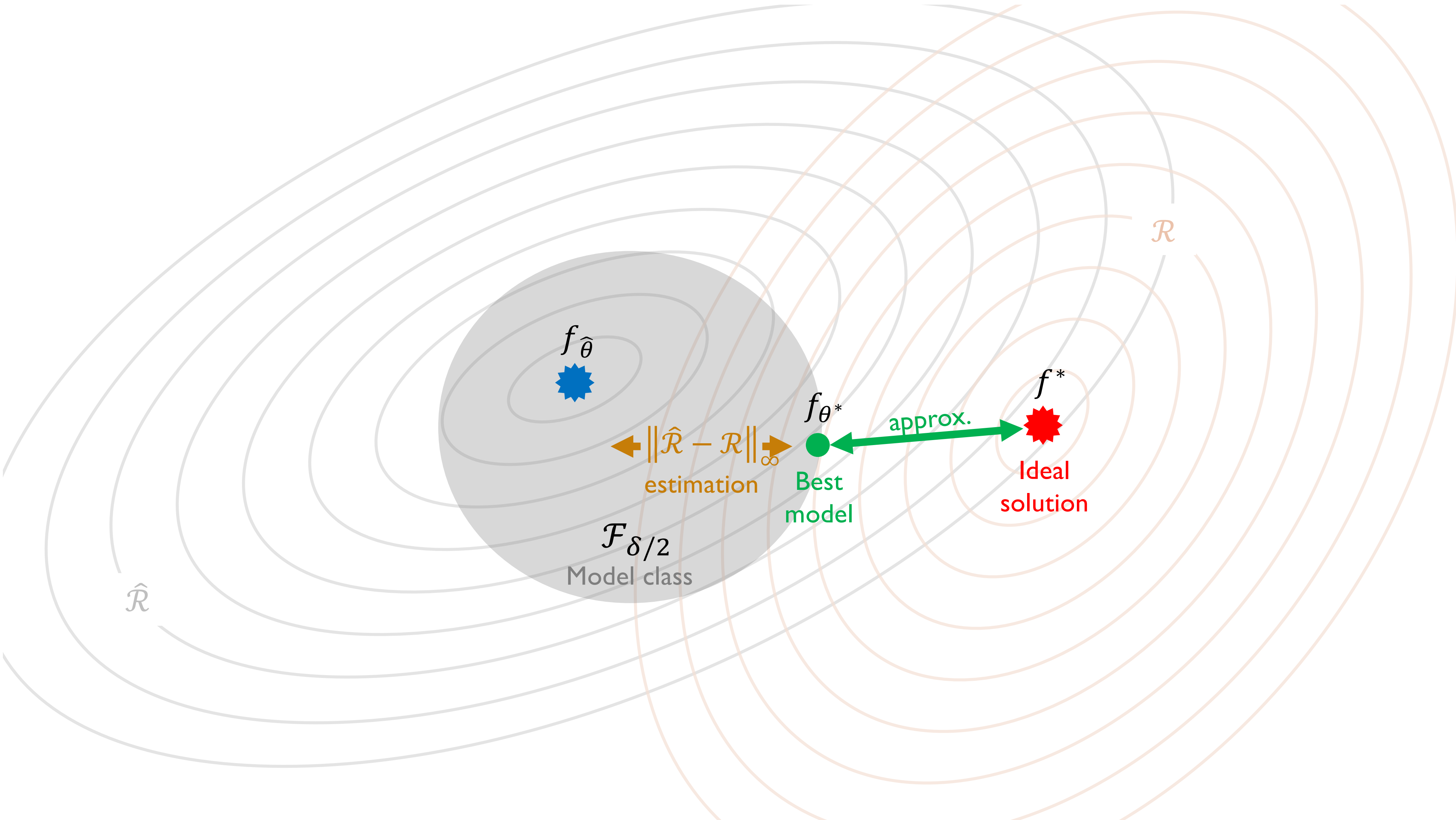
optimisation error
"how far $\hat{f}$ is from $f_{\hat{\theta}}$"

approximation error
"how expressive $\mathcal{F}_\delta$ is"


$f_{\hat{\theta}}$
$\hat{f}$
optim
$\|\hat{\mathcal{R}} - \mathcal{R}\|_\infty$
estimation
f_{θ^*}
approx.
f^*
$\mathcal{R}$
Trained estimator
Best model
Ideal solution
$\mathcal{F}_\delta$
Model class
$\hat{\mathcal{R}}$

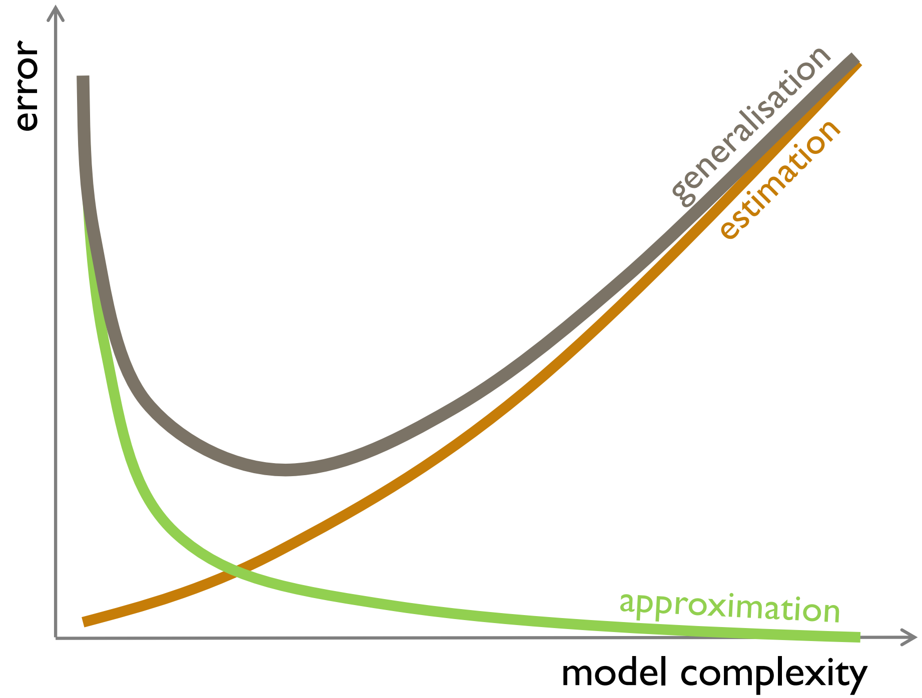


$\mathcal{R}$
$f_{\hat{\theta}}$
f^*
f_{θ^*}
approx.
$\|\hat{\mathcal{R}} - \mathcal{R}\|_\infty$
estimation
Best model
Ideal solution
$\mathcal{F}_\delta$
Model class
$\hat{\mathcal{R}}$

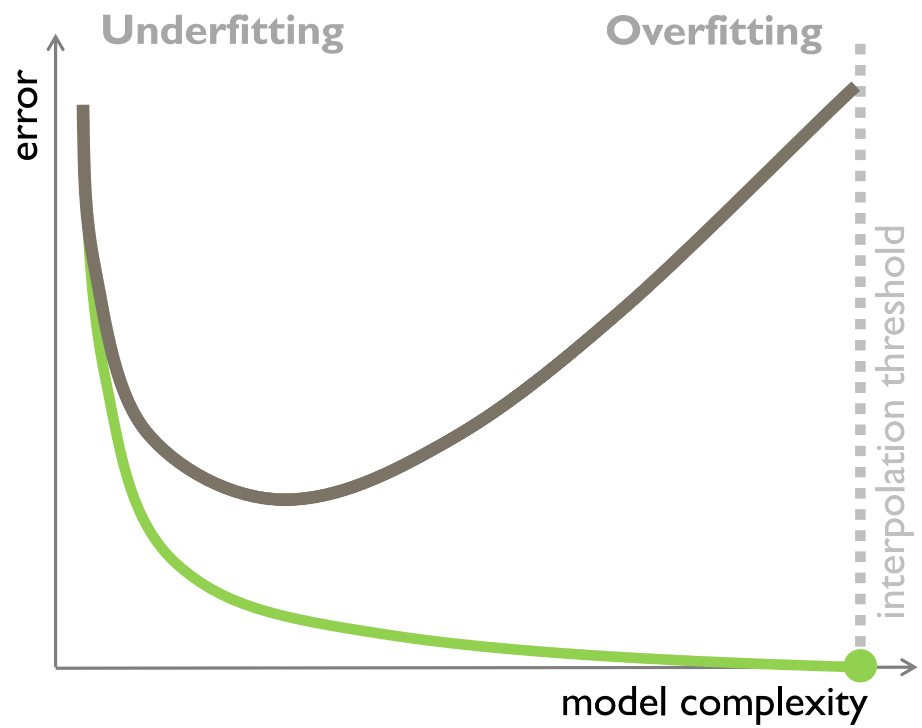


$\mathcal{R}$
$f_{\hat{\theta}}$
f^*
f_{θ^*}
approx.
$\|\hat{\mathcal{R}} - \mathcal{R}\|_\infty$
estimation
Best
model
Ideal
solution
$\mathcal{F}_{\delta/2}$
Model class
$\hat{\mathcal{R}}$

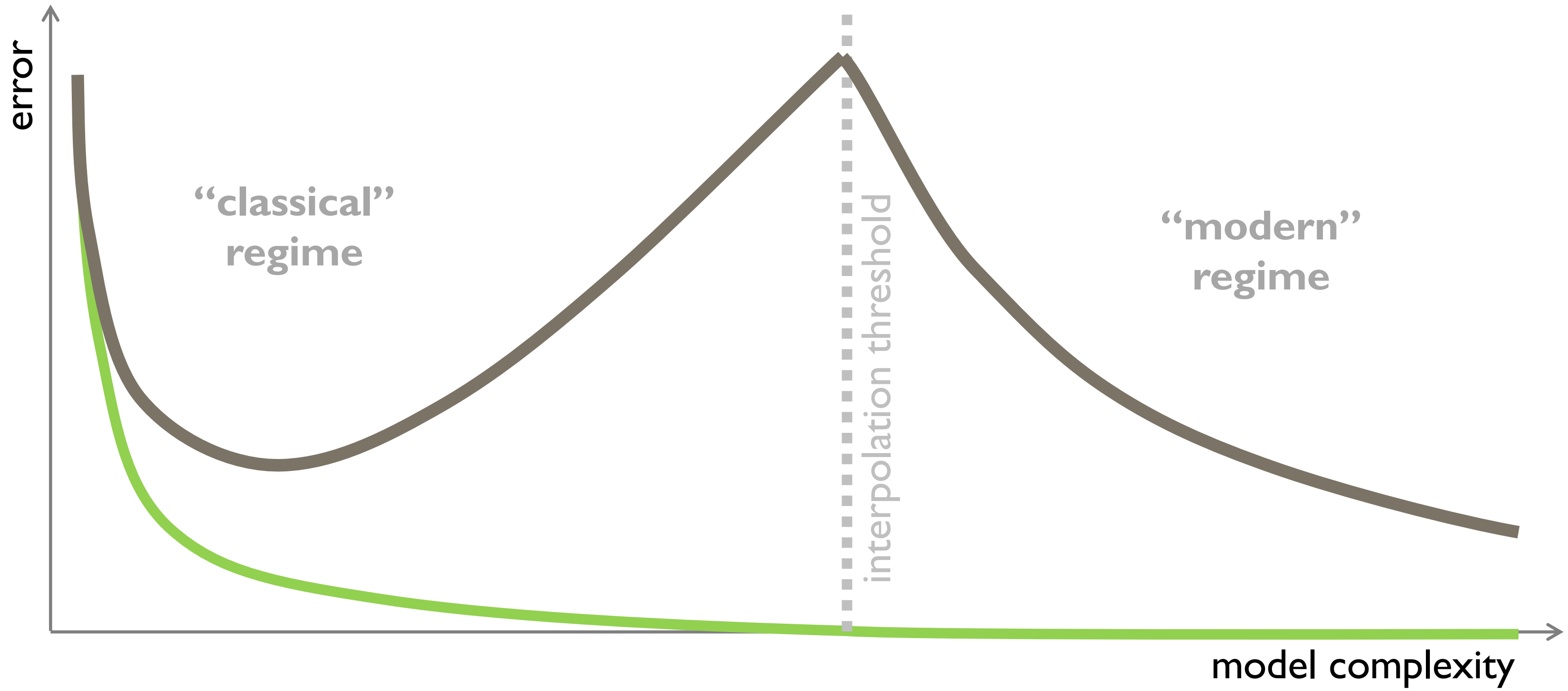
Classical Bias-Variance tradeoff



Classical Bias-Variance tradeoff



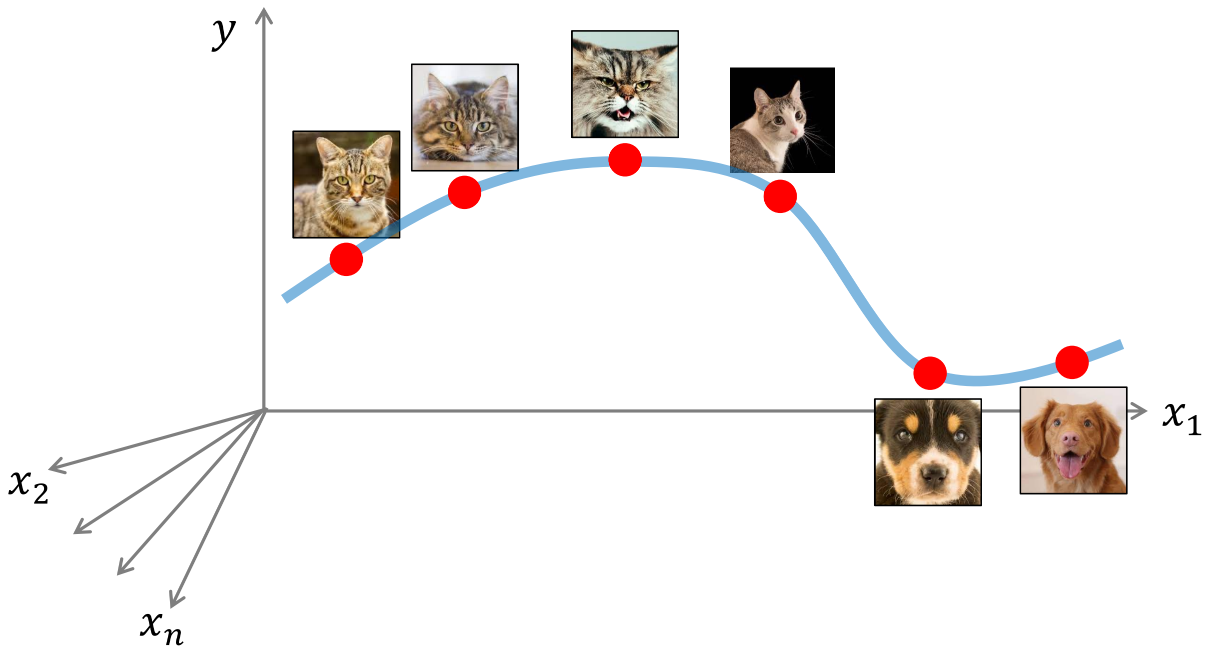
Modern Bias-Variance tradeoff: “Double Descent”



Neal et al. 2018; Belkin et al. 2019

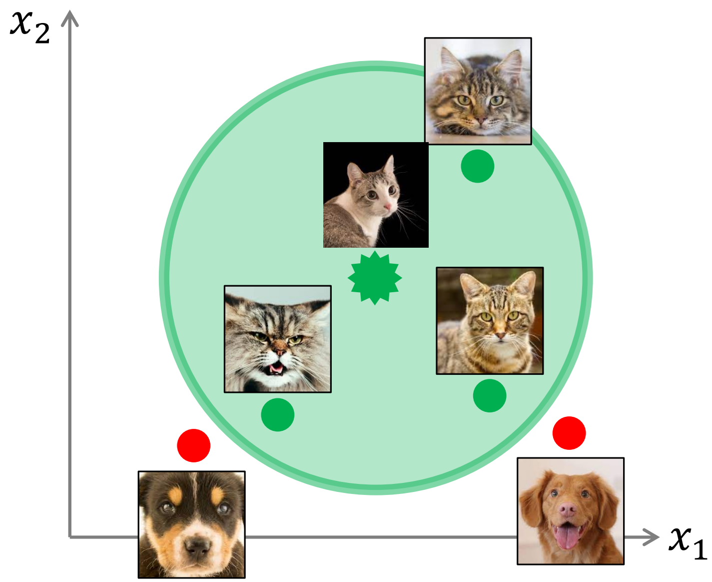
THE STORY IN HIGH DIMENSIONS

"Glorified curve fitting"



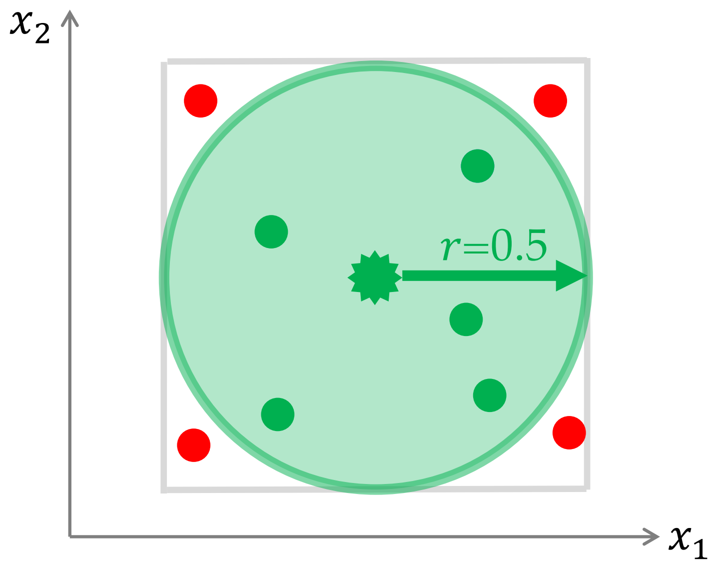
underlying assumption of function "regularity"

Nearest-neighbour classifier



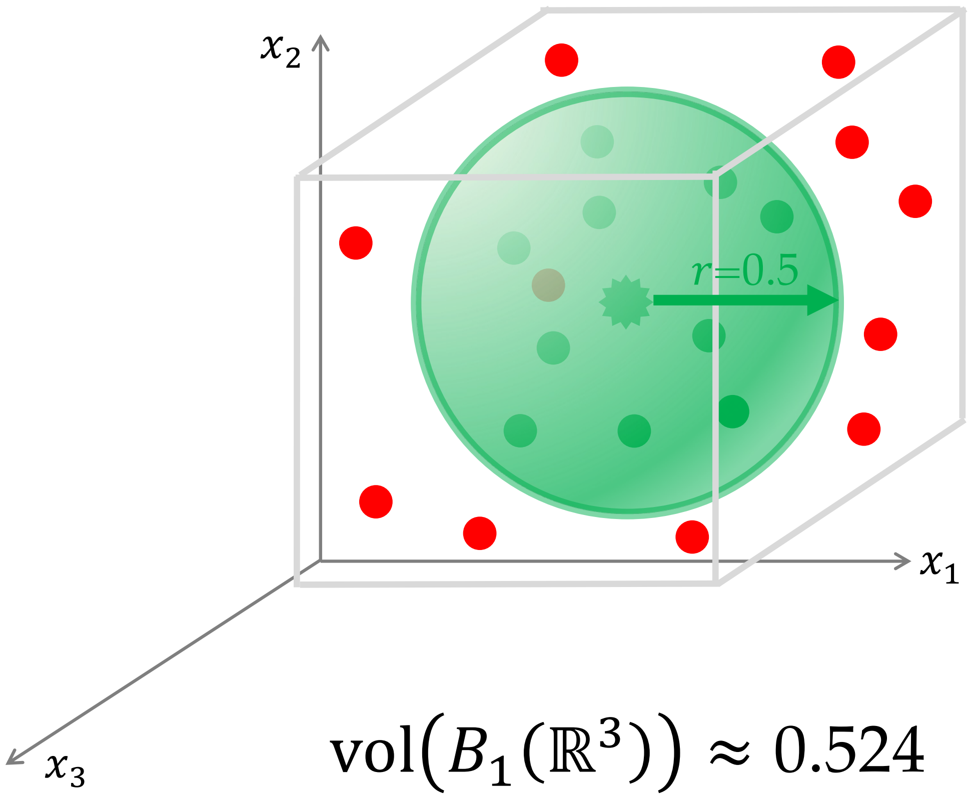
"my neighbours are similar to me"

Nearest-neighbour classifier



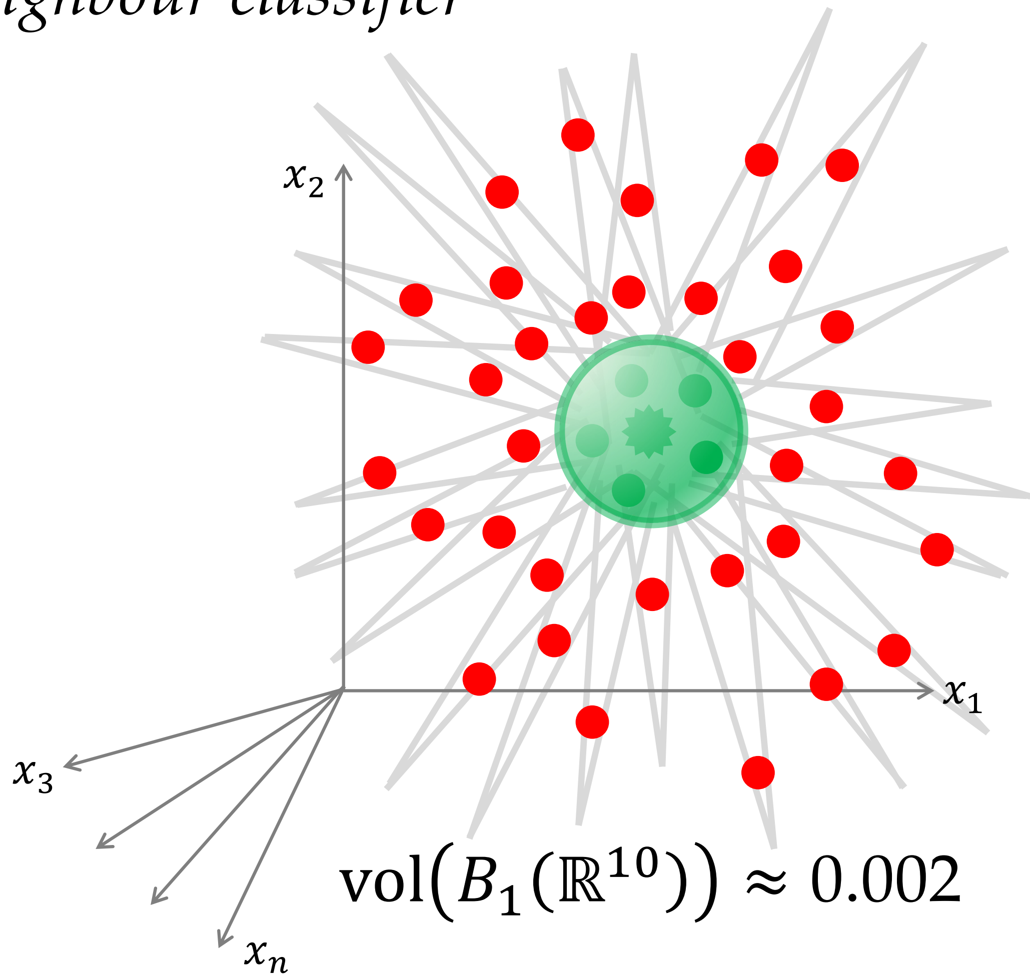
$$\mathrm{vol}\big(B_1(\mathbb{R}^2)\big) \approx 0.785$$

Nearest-neighbour classifier



$$\mathrm{vol}\big(B_1(\mathbb{R}^3)\big) \approx 0.524$$

Nearest-neighbour classifier



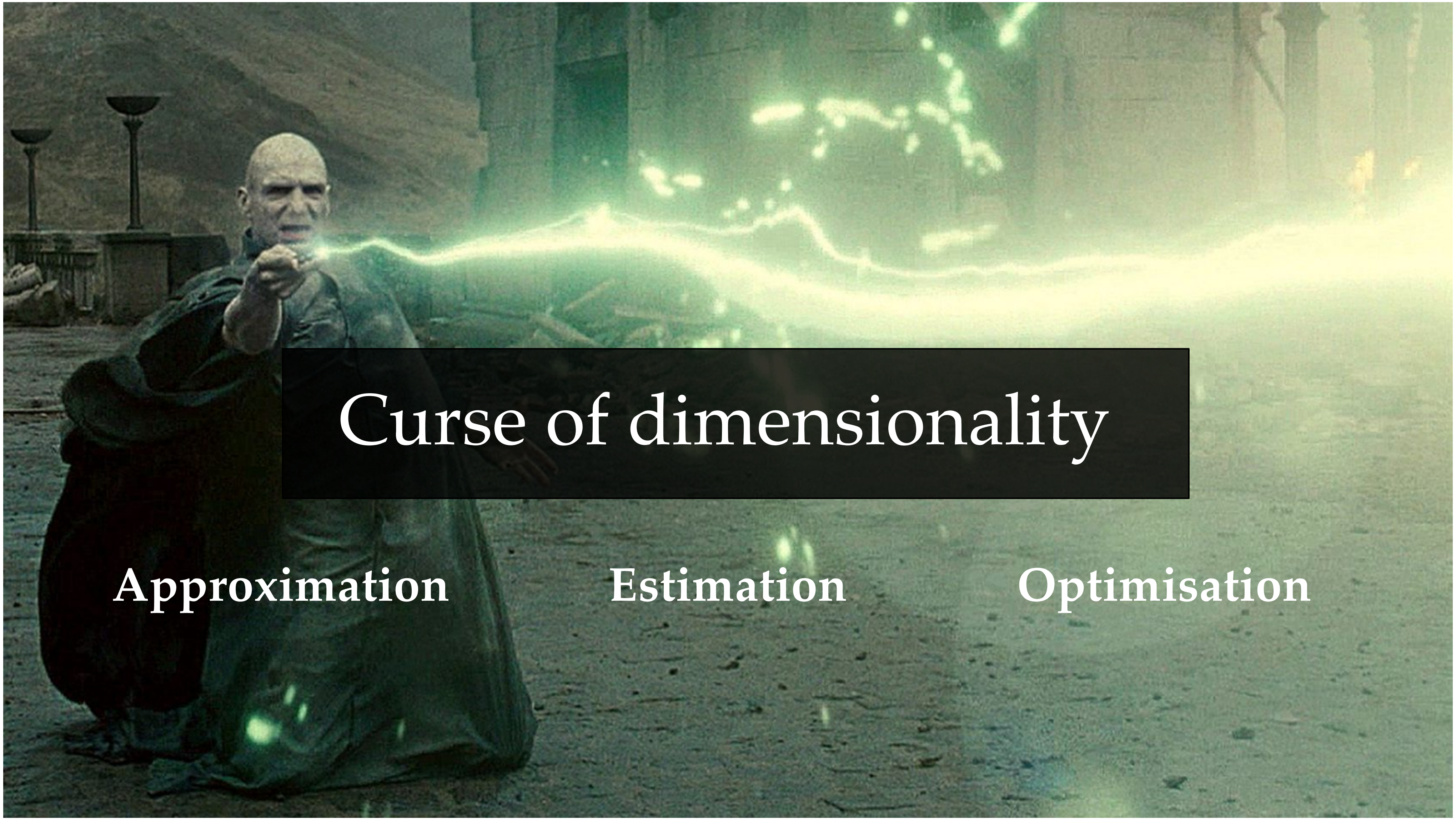
$$\mathrm{vol}\big(B_1(\mathbb{R}^{10})\big) \approx 0.002$$

"[dimensionality is] a curse which has hung over the head of the physicist and astronomer for many a year. "

— *Dynamic Programming*

R. Bellman

Bellman 1957


Curse of dimensionality
Approximation
Estimation
Optimisation

CURSE IN ESTIMATION

Learning Lipschitz functions

- A function $f: \mathcal{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ is **$\boldsymbol{\beta}$-Lipschitz** if $|f(x) - f(x')| \leq \beta \|x - x'\|$
  - $\beta = \mathrm{Lip}(f)$ is the *Lipschitz constant* of f
  - Strong form of uniform continuity
  - Global property (unlike simple continuity)

Reminder:
f is **continuous** at x if $\forall \varepsilon > 0 \;\; \exists \delta > 0$ s.t. $\forall x' \;\; \|x - x'\| < \delta \implies |f(x) - f(x')| < \varepsilon.$
f is **uniformly continuous** if $\forall \varepsilon > 0 \;\; \exists \delta > 0$ s.t. $\forall x, x' \;\; \|x - x'\| < \delta \implies |f(x) - f(x')| < \varepsilon.$

Learning Lipschitz functions

- A function $f : \mathcal{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ is $\boldsymbol{\beta}$**-Lipschitz** if $|f(x) - f(x')| \leq \beta \|x - x'\|$
    - $\beta = \mathrm{Lip}(f)$ is the *Lipschitz constant* of f
    - Strong form of uniform continuity
    - Global property (unlike simple continuity)

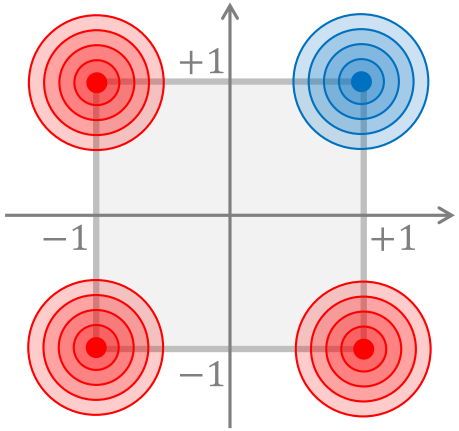
How many samples N are needed to approximate a Lipschitz function in $\mathbb{R}^d$ with accuracy ε?

Learning Lipschitz functions: Lower bound

- Consider a 1-Lipschitz function constructed as a superpositions of blobs placed at the corners $H_d = \{(z_1, \dots, z_d) : z_i = \pm 1\}$ of a d-dimensional hypercube

$$f(x) = \sum_{z \in H_d} c_z \varphi(x - z) \qquad c_z = \pm 1$$

- Assume f is sampled at N samples



Exercise: prove that if $N \ll 2^d$ then any estimator $\hat{f}$ will incur a relative error of $\frac{\mathbb{E}|f - \hat{f}|^2}{\mathbb{E}|f|^2} = \Theta(1)$

Von Luxburg, Bosquet 2004

Learning Lipschitz functions: Lower bound

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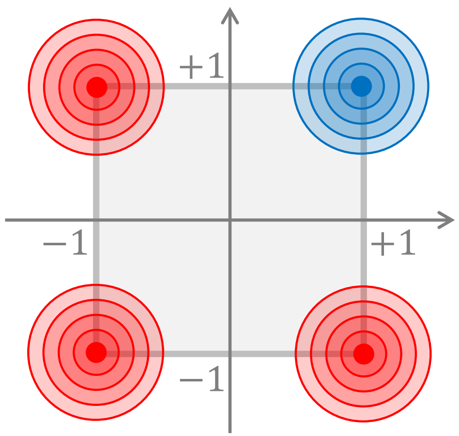
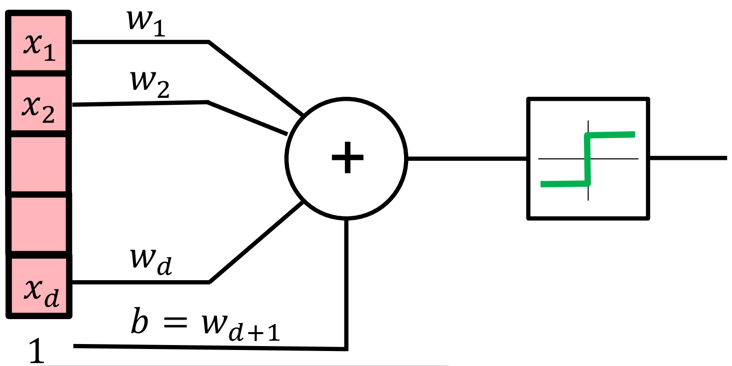


Learning Lipschitz functions is a dimensionality-cursed problem

Von Luxburg, Bosquet 2004

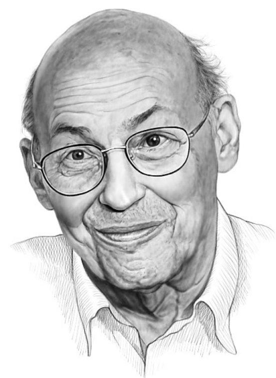
CURSE IN APPROXIMATION

Simple Perceptrons

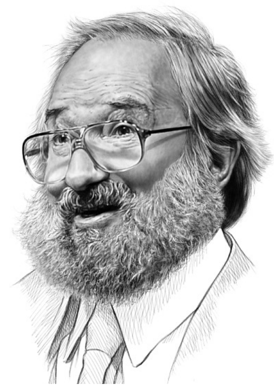


$$y = \mathrm{sign}(\mathbf{w}^{\mathrm{T}}\mathbf{x})$$

F. Rosenblatt



M. Minsky

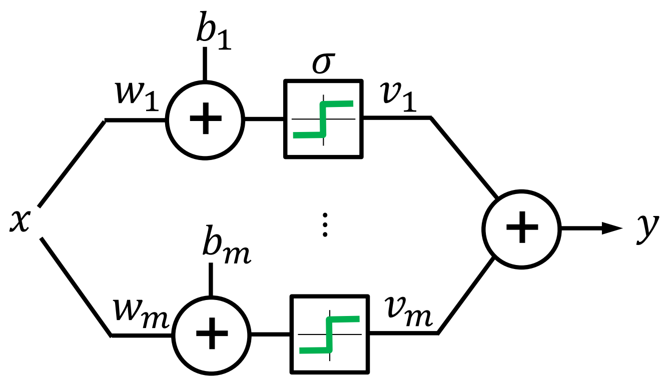


S. Papert

Shallow Perceptrons

- **Two-layer perceptron** with a non-polynomial activation function σ

$$\mathcal{F} = \left\{ f(x) = \sum_{j \le m} v_j \sigma(w_j^{\mathrm{T}} x + b_j) \right\}$$



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- Parametrised by weights $\mathbf{W}, \mathbf{b}, \mathbf{v}$
- Various definitions of capacity, e.g.
  - *Number of neurons:* $\gamma(f) = m$
  - *Path norm:* $\gamma(f) = \sum |v_j| \left(\|w_j\| + |b_j| \right)$

Shallow Perceptrons are universal approximators

- **Two-layer perceptron** with a non-polynomial activation function σ

$$\mathcal{F} = \left\{ f(x) = \sum_{j \leq m} v_j \sigma(w_j^{\mathrm{T}} x + b_j) \right\}$$

> **Universal Approximation Theorem:** $\mathcal{F}$ is *dense* in the class of continuous d-dimensional functions w.r.t. the uniform compact topology

$A \subseteq X$ is **dense** in X if $\bar{A} = X$, where $\bar{A} = A \cup \{\lim_{n\to\infty} a_n : a_n \in A\}$

G. Cybenko

K. Hornik

Hilbert 1990 (Thirteenth Problem); Kolmogorov 1956; Arnold 1957 ("Superposition Theorem"); Hecht-Nielsen 1987 (first use in neural networks)
Cybenko 1989; Funahashi 1989; Hornik et al. 1989; Barron 1993; Leshno et al. 1993; Maiorov 1999; Pinkus 1999

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Universal Approximation Theorem: $\mathcal{F}$ can uniformly approximate any continuous d-dimensional function on a compact set to any desired accuracy ε.

G. Cybenko

K. Hornik

Hilbert 1990 (Thirteenth Problem); Kolmogorov 1956; Arnold 1957 (“Superposition Theorem”); Hecht-Nielsen 1987 (first use in neural networks)
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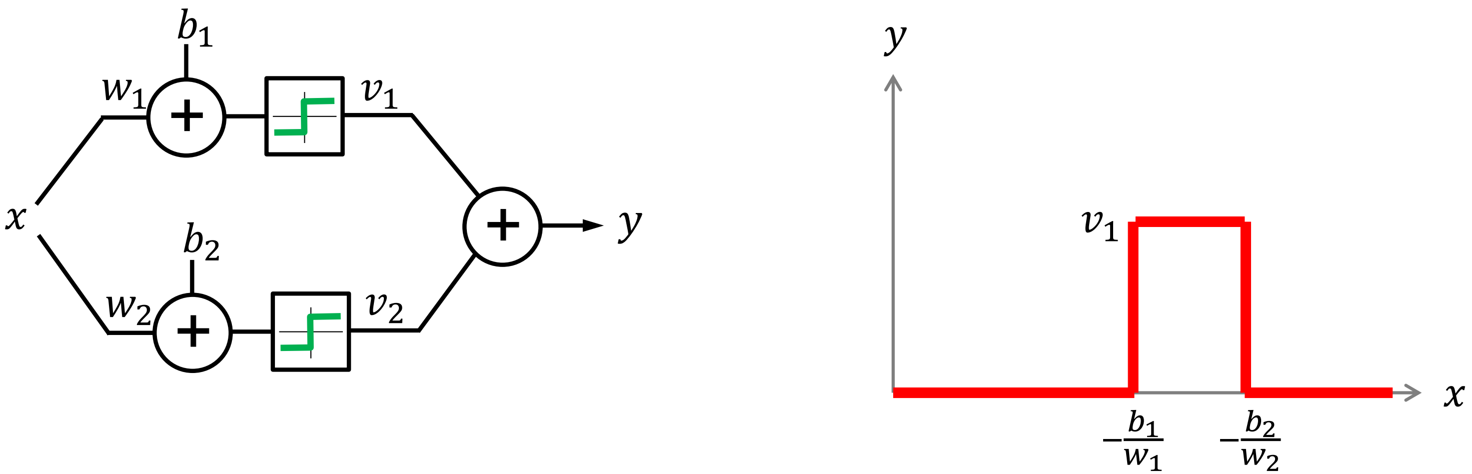

Shallow Perceptrons are universal approximators

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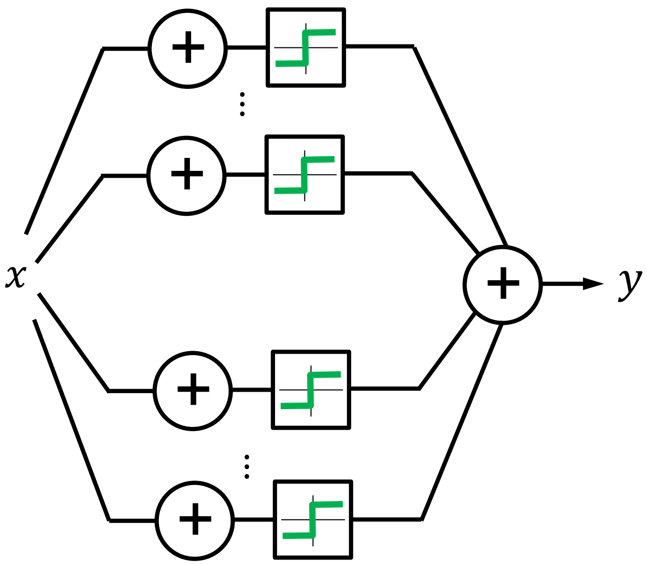

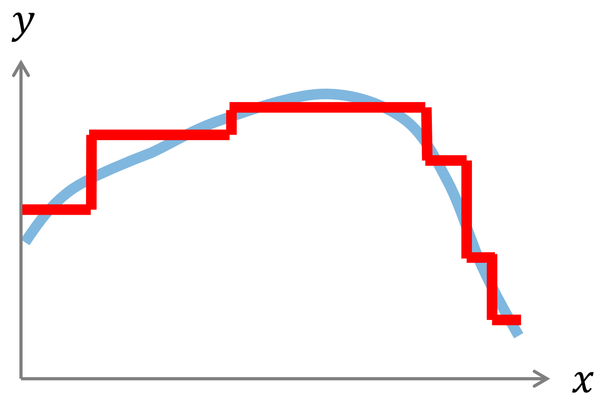

Shallow Perceptrons are universal approximators

Universal Approximation Theorem: σ is not polynomial iff for every continuous function $f: K \subset \mathbb{R}^d \to \mathbb{R}$ defined on a *compact set* K and $\varepsilon > 0$, there exists a two-layer Perceptron with m neurons and weights $\mathbf{W}, \mathbf{b}, \mathbf{v}$ s.t.

$$\max_{x \in K} \left| f(x) - \sum_{j \le m} v_j \sigma(w_j^{\mathrm{T}} x + b_j) \right| < \varepsilon$$

- Fixed number of layers (*"bounded depth"*)
- Does not tell how many neurons m are needed (*"arbitrary width"*)
- Existence result: does not tell *how* to find the weights
- There are stronger results, including bounded depth and width

Cybenko 1989; Hornik 1991; Pinkus 1999

Shallow Perceptrons are universal approximators

Universal Approximation Theorem: σ is not polynomial iff for every continuous function $f: K \subset \mathbb{R}^d \to \mathbb{R}$ defined on a *compact set* K and $\varepsilon > 0$, there exists a two-layer Perceptron with m neurons and weights $\mathbf{W}, \mathbf{b}, \mathbf{v}$ s.t.

$$\max_{x \in K} \left| f(x) - \sum_{j \le m} v_j \sigma(w_j^{\mathrm{T}} x + b_j) \right| < \varepsilon$$

What is the relation between dimension d, number of neurons m, and the error ε?

Cybenko 1989; Hornik 1991

Approximation rates

- Bound on the approximation error

$$\varepsilon = \inf_{g \in \mathcal{F}} \sup_{x \in K \subset \mathbb{R}^d} |f(x) - g(x)|$$

w.r.t. d, m for different classes of functions

- *Sobolev class* $f \in H^s(\mathbb{R}^d) = \left\{ f \in L_2(\mathbb{R}^d) : \int_{\mathbb{R}^d} (1 + \|\omega\|^2)^s \left|\hat{f}(\omega)\right|^2 \mathrm{d}\omega < \infty \right\}$

  error is exponential $\varepsilon = \mathcal{O}\left(m^{-s/d}\right)$ **dimensionality-cursed!**

  "functions with sufficiently many derivatives"

Maiorov 1999

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- *Barron class* $\quad f \in \left\{ f \in L_2(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|\omega\|^2 \left|\hat{f}(\omega)\right|^2 \mathrm{d}\omega < \infty \right\}$

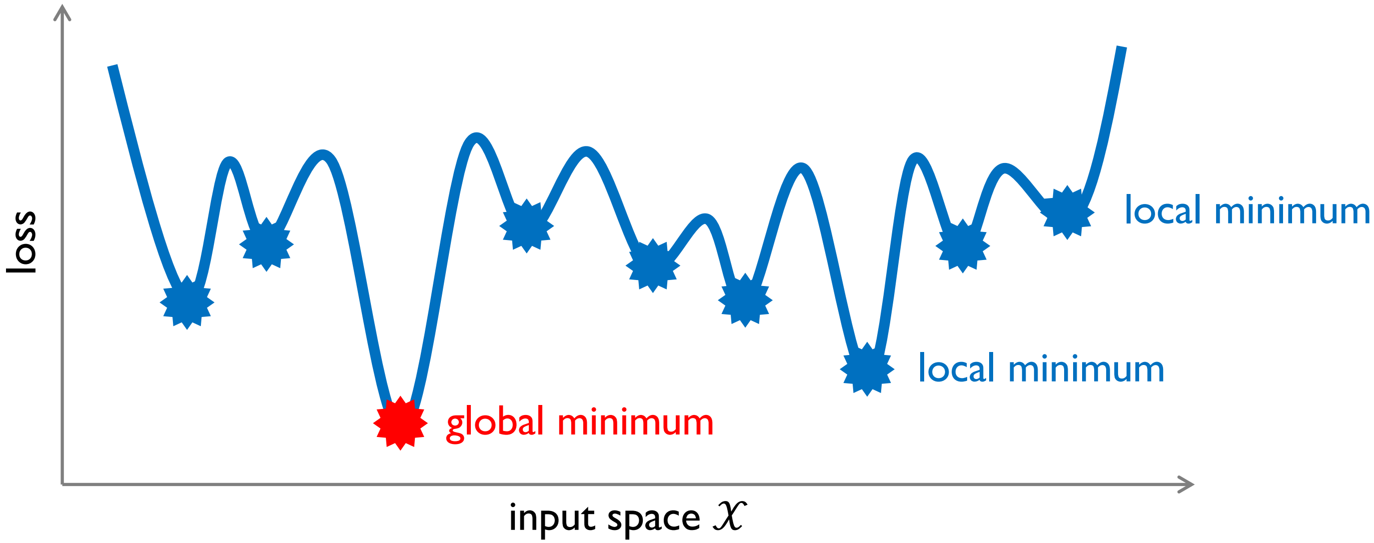
  error is $\varepsilon = \mathcal{O}(m^{-1})$ **too strong assumption in practice!**

Maiorov 1999; Barron 1993

CURSE IN OPTIMISATION

How hard is optimisation in high dimensions?

- Finding a global optimum of a generic high-dimensional function is NP-hard



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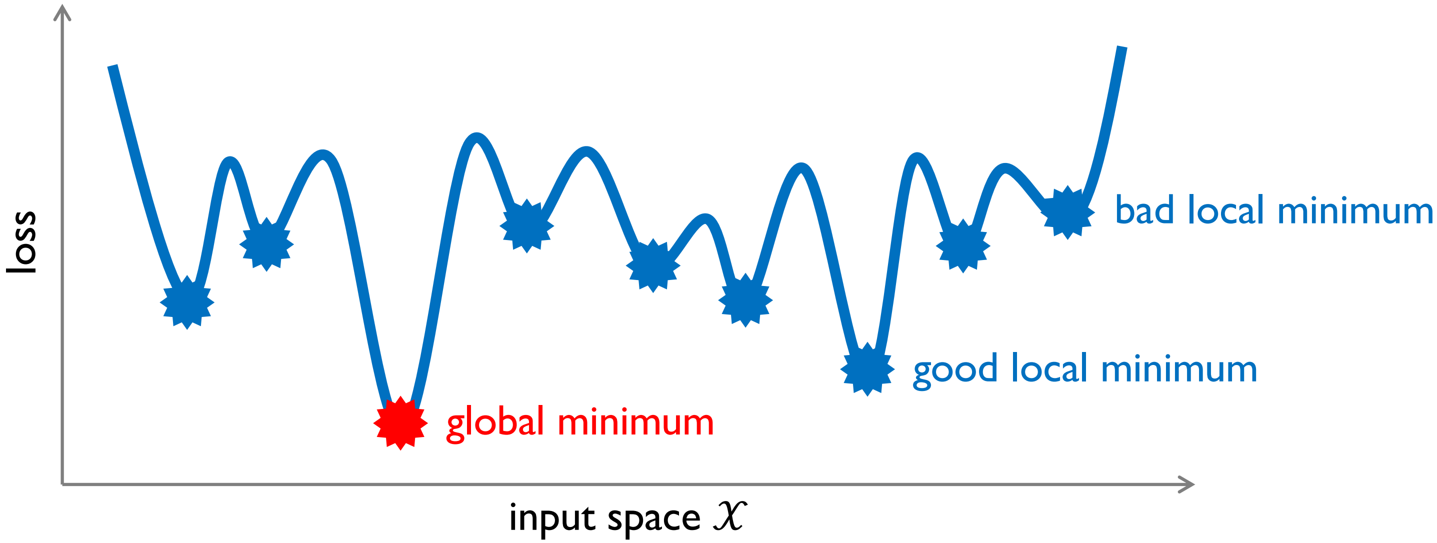
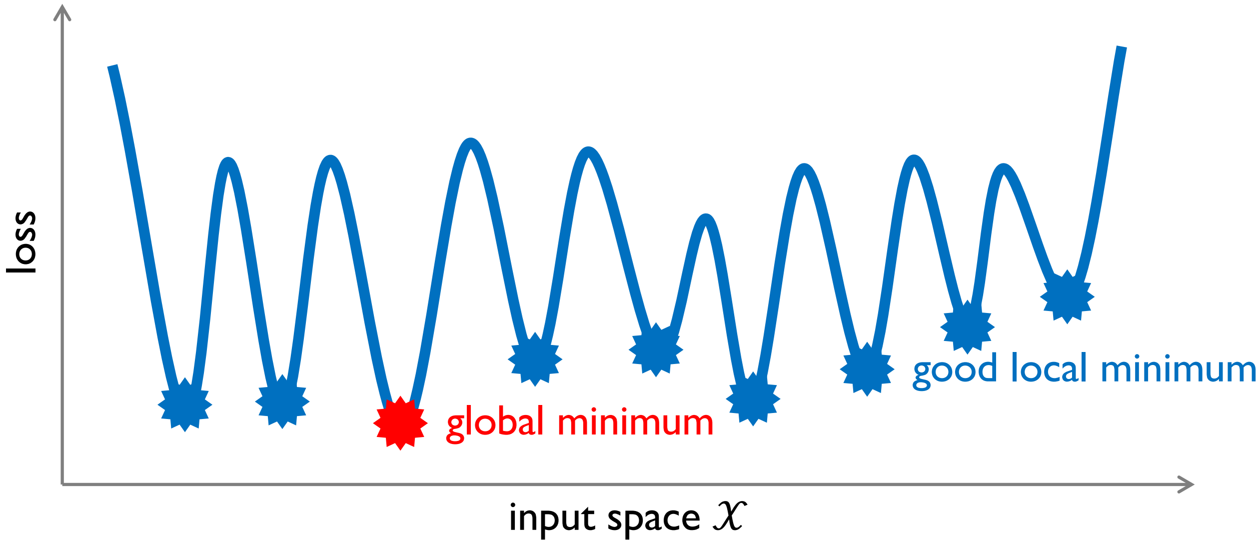


How hard is optimisation in high dimensions?

- Finding a global optimum of a generic high-dimensional function is NP-hard
- Deep neural networks have more benign landscapes with no "bad local minima"



How hard is optimisation in high dimensions?

- Finding a global optimum of a generic high-dimensional function is NP-hard
- Deep neural networks have more benign landscapes with no “bad local minima”
  - Most local minima are equivalent and yield similar test performance
  - The probability of finding a “bad” local minimum decreases with network depth
  - Finding the global minimum on the training set (as opposed to one of the many good local ones) is not useful in practice and may lead to overfitting

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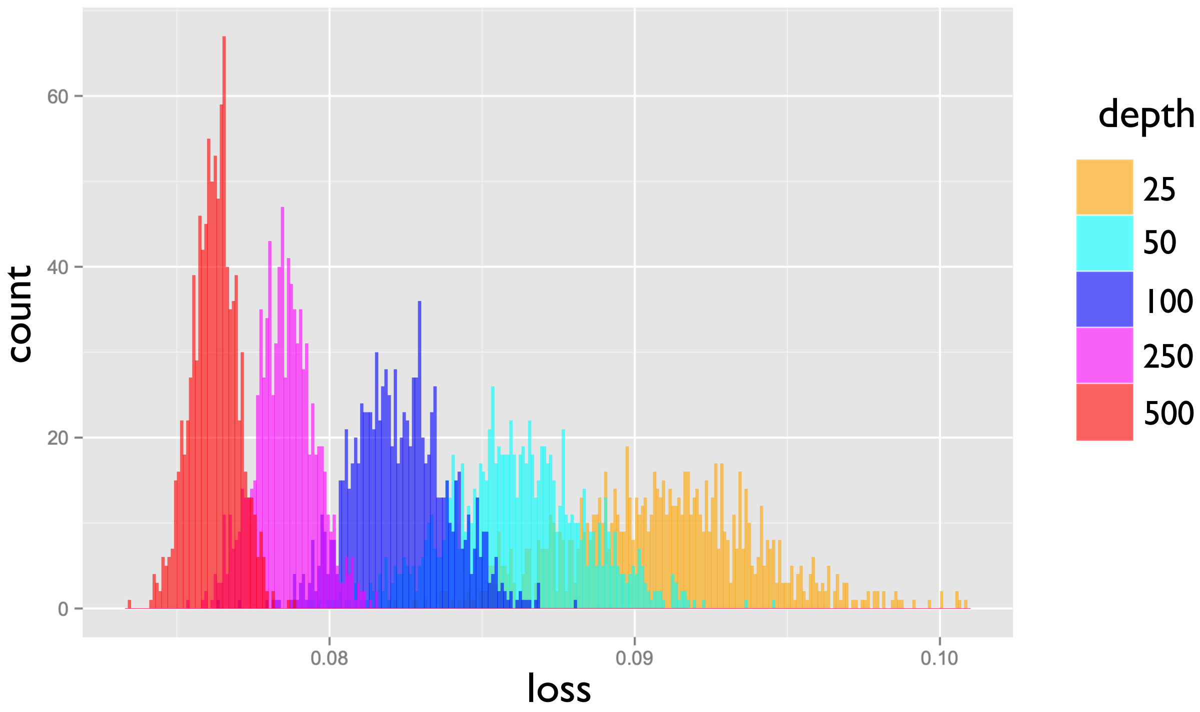

Choromanska et al. 2015

How hard is optimisation in high dimensions?

- Finding a global optimum of a generic high-dimensional function is NP-hard
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  - The probability of finding a “bad” local minimum decreases with network depth
  - Finding the global minimum on the training set (as opposed to one of the many good local ones) is not useful in practice and may lead to overfitting
- Gradient descent can efficiently find local minima in high dimension

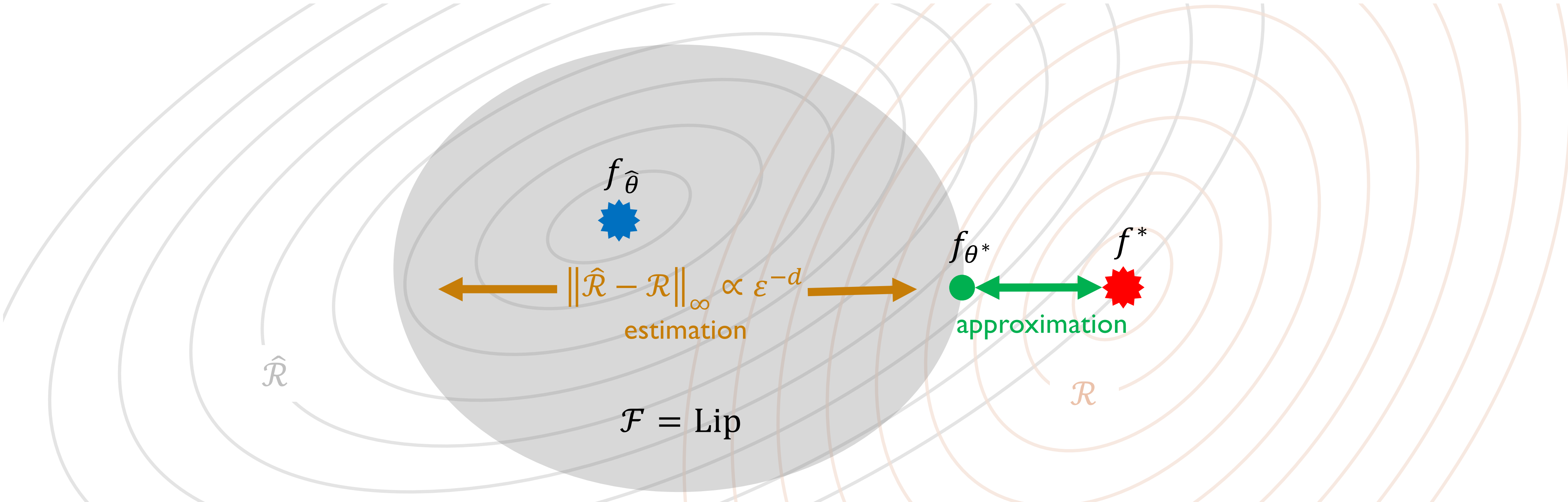
> **Typical result:** Noisy gradient descent can find ε-approximate second-order stationary points of a β-smooth loss function in $\tilde{O}(\beta \log d/\varepsilon^2)$ iterations.

Jin 2017

GEOMETRIC REGULARITY

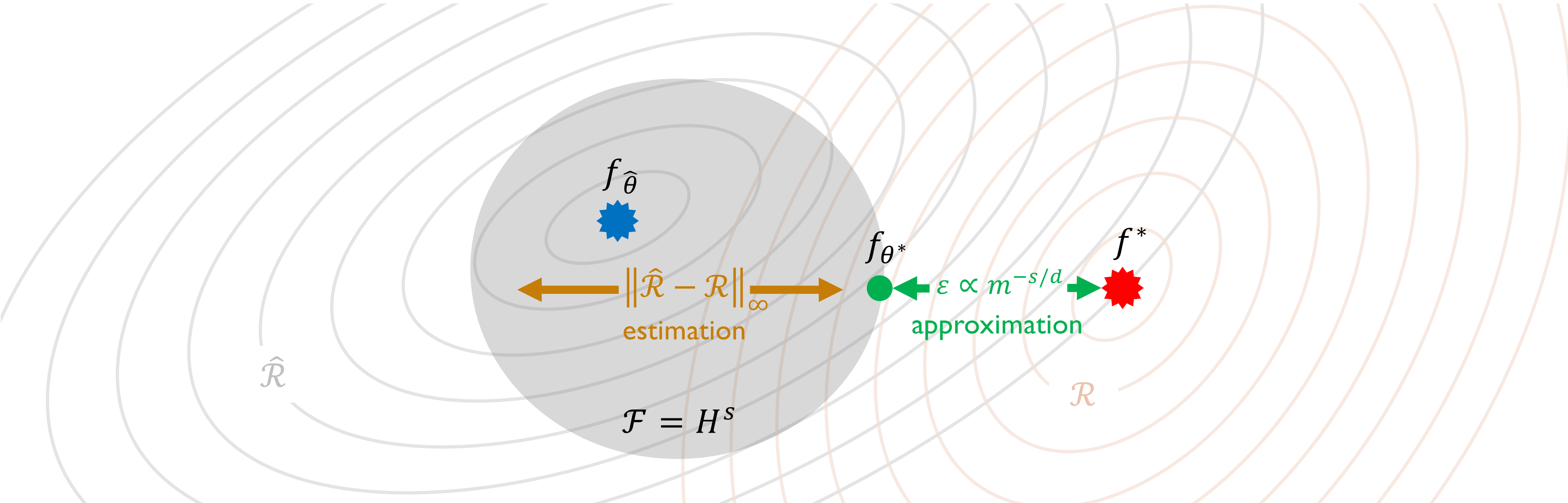
Findings so far: classical notions of regularity are of little use!

- Lipschitz class is too large: estimation error is dimensionality-cursed

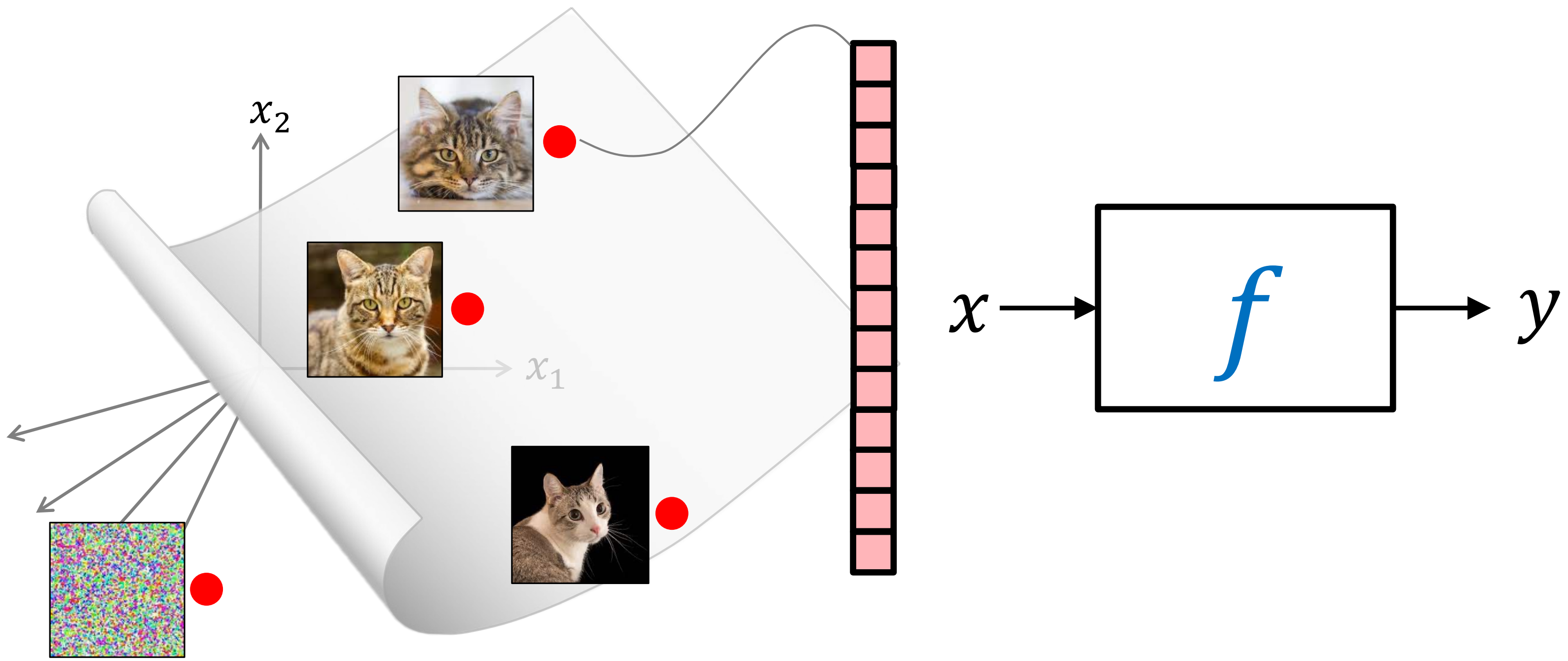


Findings so far: classical notions of regularity are of little use!

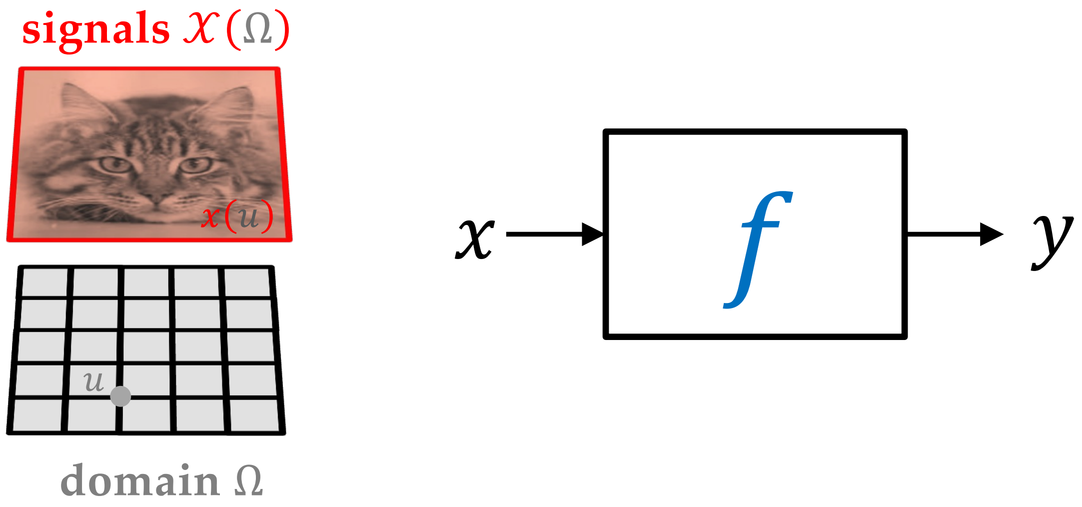
- Lipschitz class is too large: estimation error is dimensionality-cursed
- Sobolev class is too small: approximation error is dimensionality-cursed



Geometric priors



Geometric priors



Takeaways

- Learning in high dimensions is plagued by the *curse of dimensionality*
- Impossible without assumptions ("priors")
- Classical assumptions of regularity (from low-dimensional analysis) are not appropriate priors
- *Geometric priors:* inputs are signals defined over low-dimensional geometric domains
- Next lectures: how to incorporate geometric priors into neural network architectures *("Geometric Deep Learning")*

Key Concepts

- Approximation, Estimation & Optimisation errors
- Bias-Variance tradeoff
- Curse of dimensionality
- Universal approximation

Main References

- M. Bronstein et al., Geometric deep learning, *arXiv:2104.13478, 2021*. Section 2 "Learning in high dimensions"
- O. Bosquet, S. Boucheron, G. Lugosi, Introduction to statistical learning theory, *Lecture Notes in Computer Science* 3176, Springer, 2004. Basics of statistical ML
- U. von Luxburg, O. Bosquet, Distance-based classification with Lipschitz functions, *JMLR* 5:669–695, 2004. Bounds for Lipschitz functions
- A. Pinkus, Approximation theory of the MLP model in neural networks, *Acta Numerica* 8:143–195, 1999. Universal approximation results for neural networks

Background Pre-Read

- A. Bronstein, Probability and statistics: a survival guide, Course notes. Refresher of probability & statistics for ML