KU LEUVEN

Function Approximation with Numerical Redundancy

Astrid Herremans
joint work with Daan Huybrechs

NUMA fwo

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$$f \approx \sum_{i=1}^{n} c_i \, \phi_i$$

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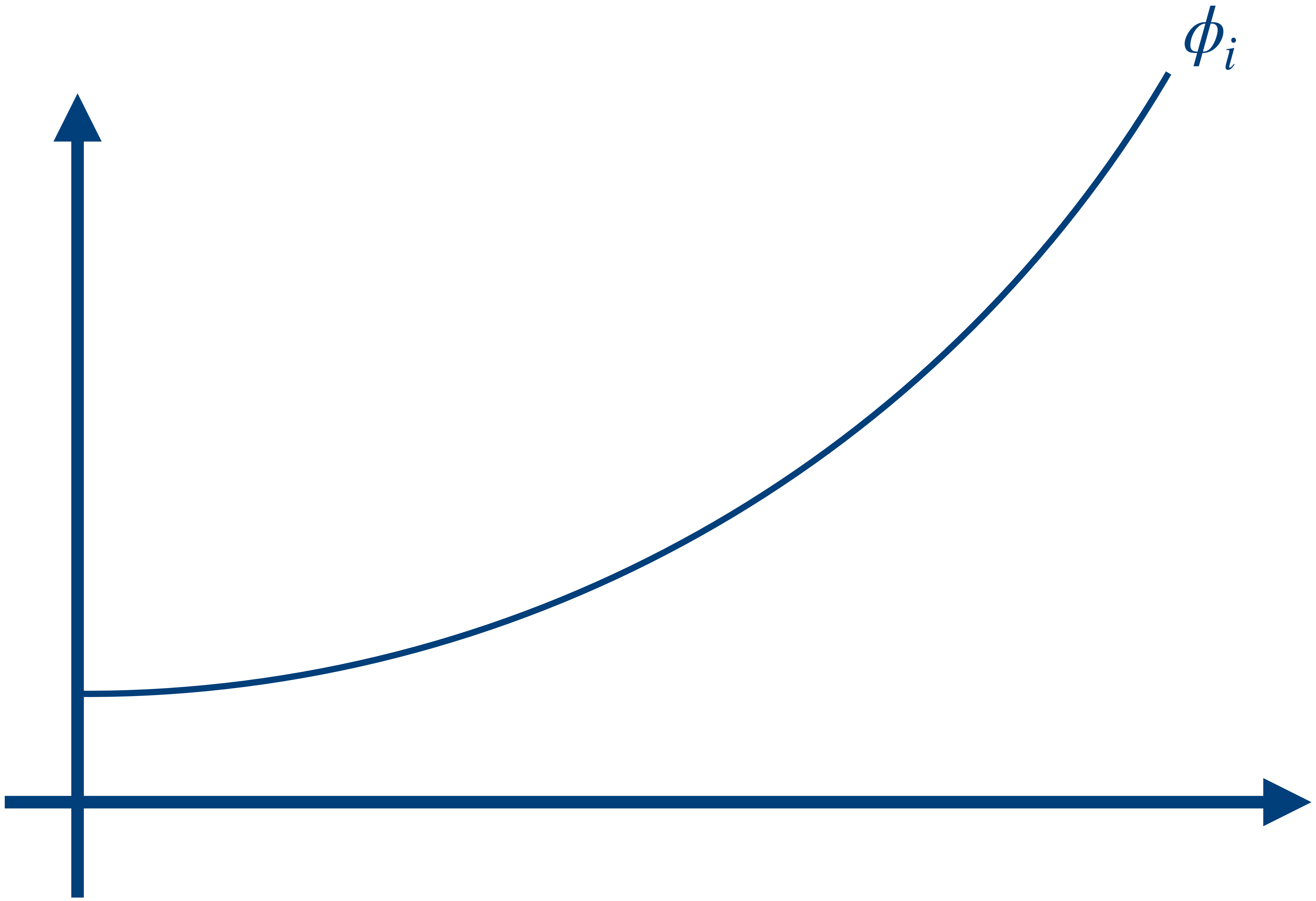
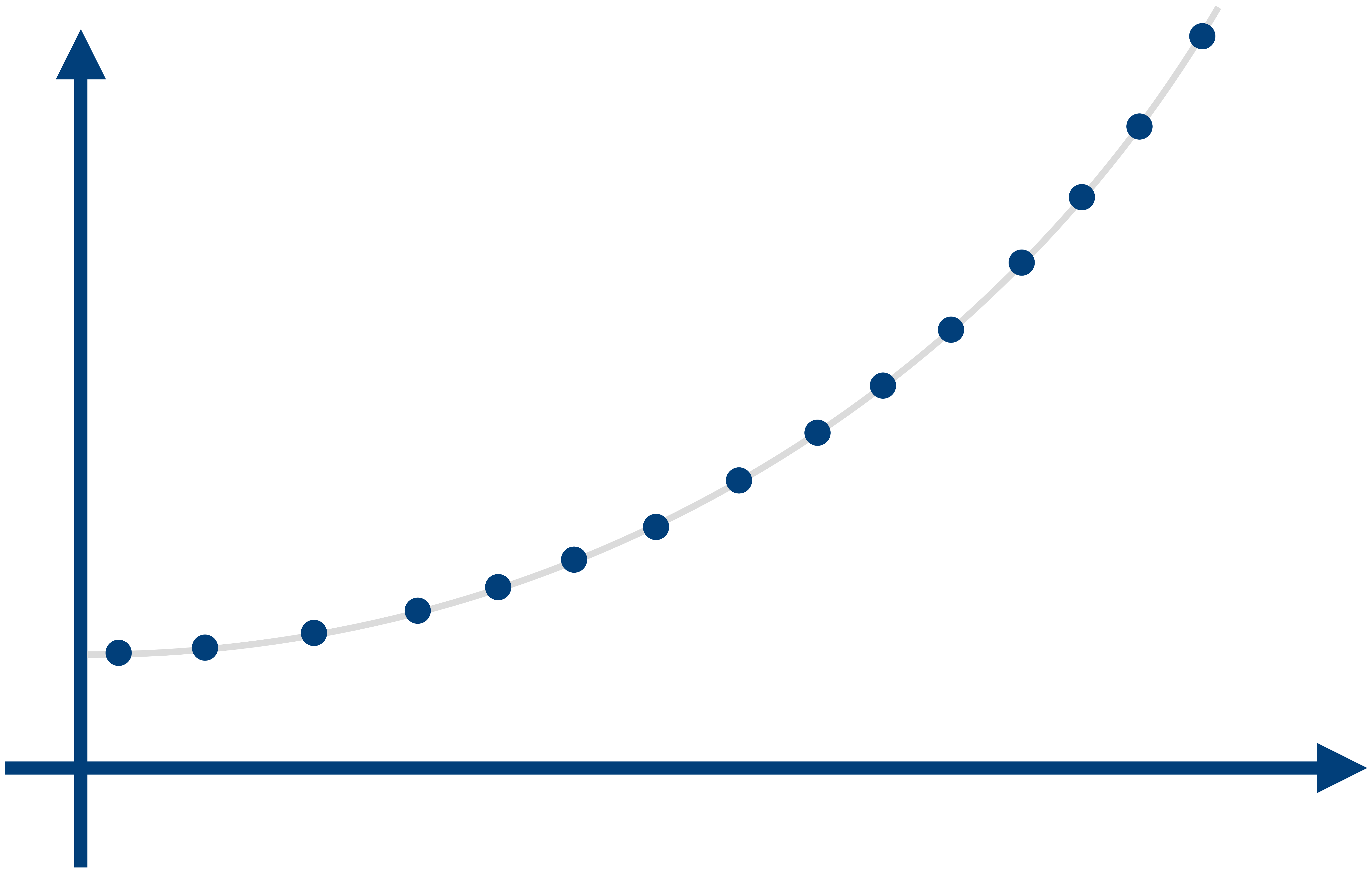
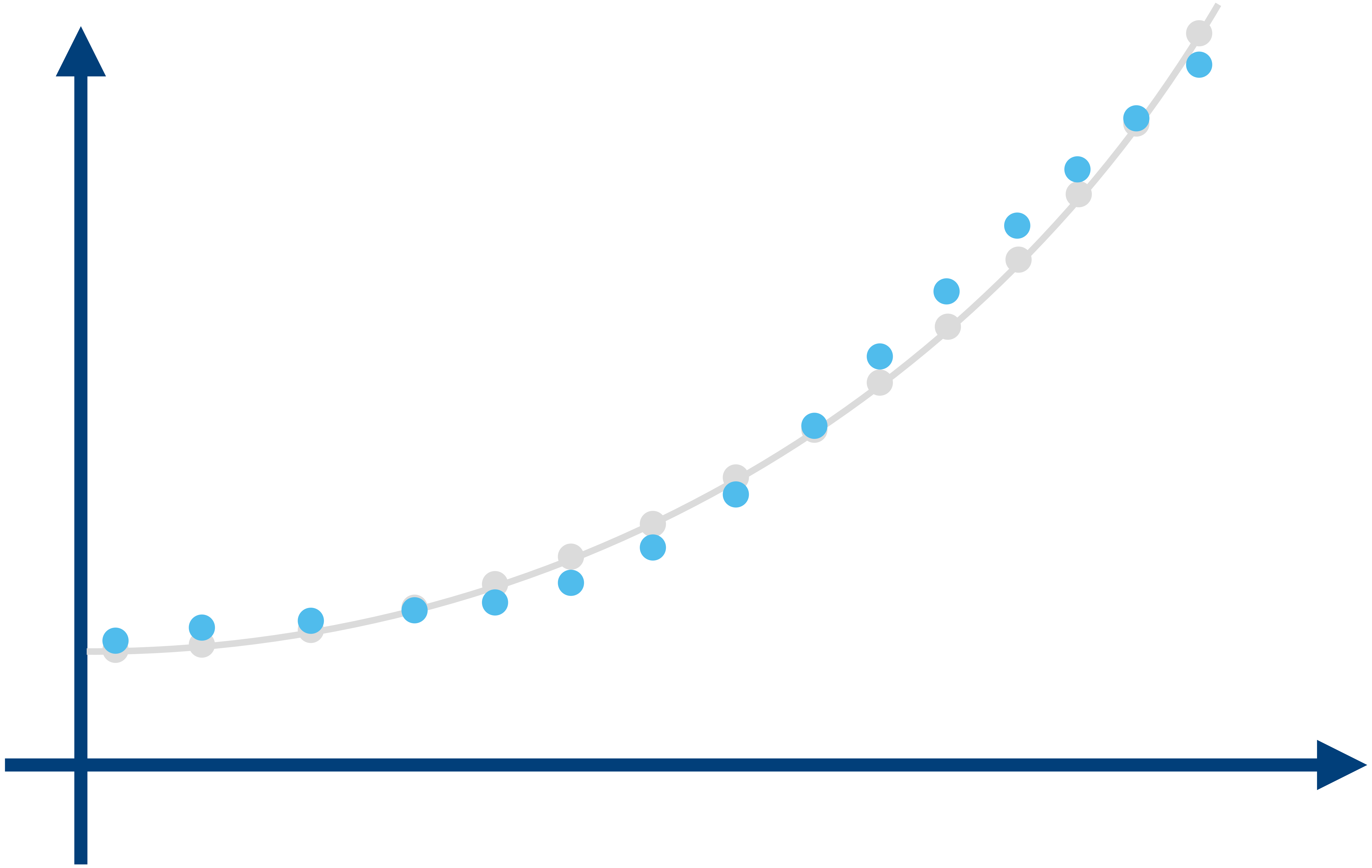
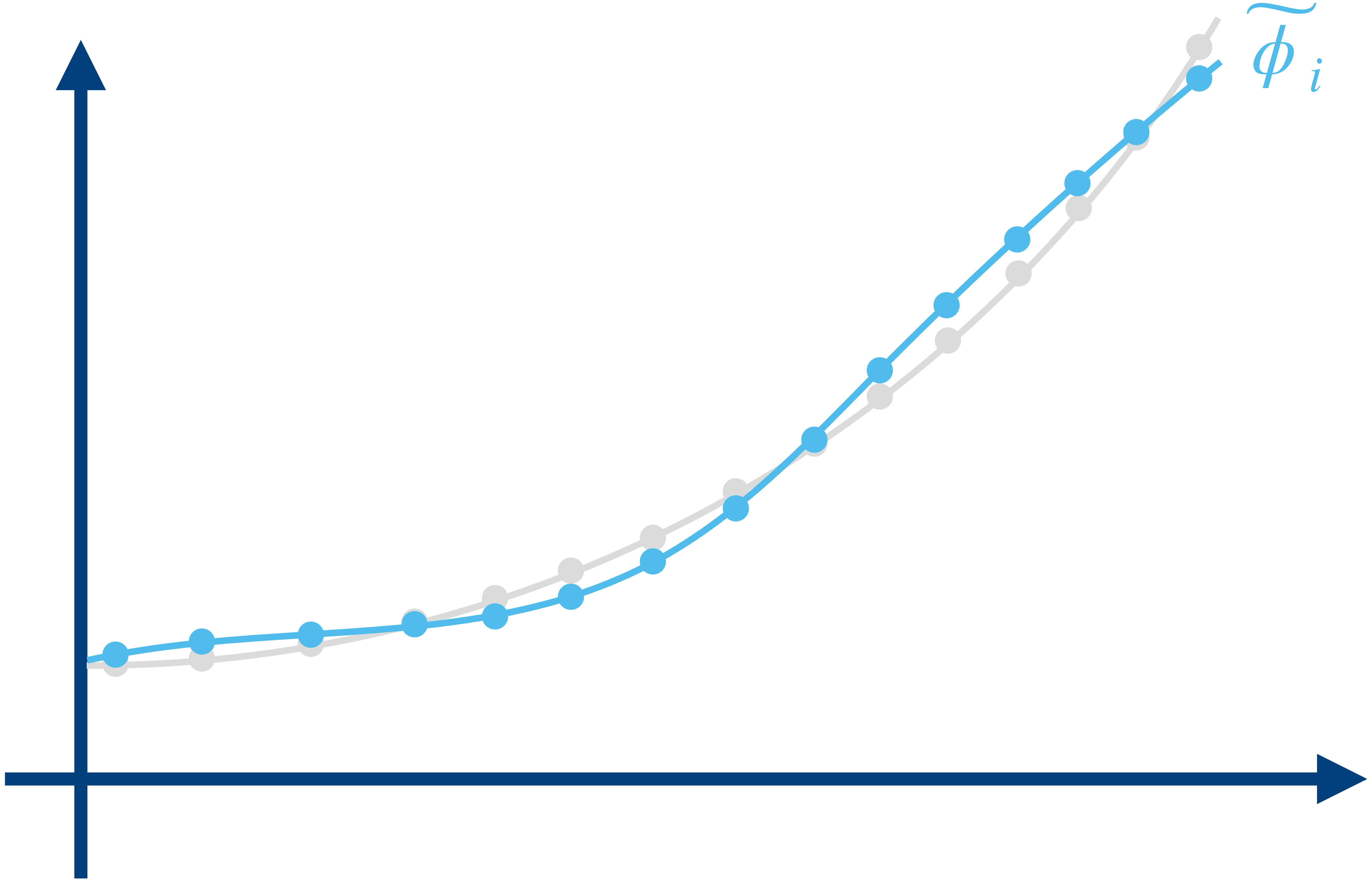
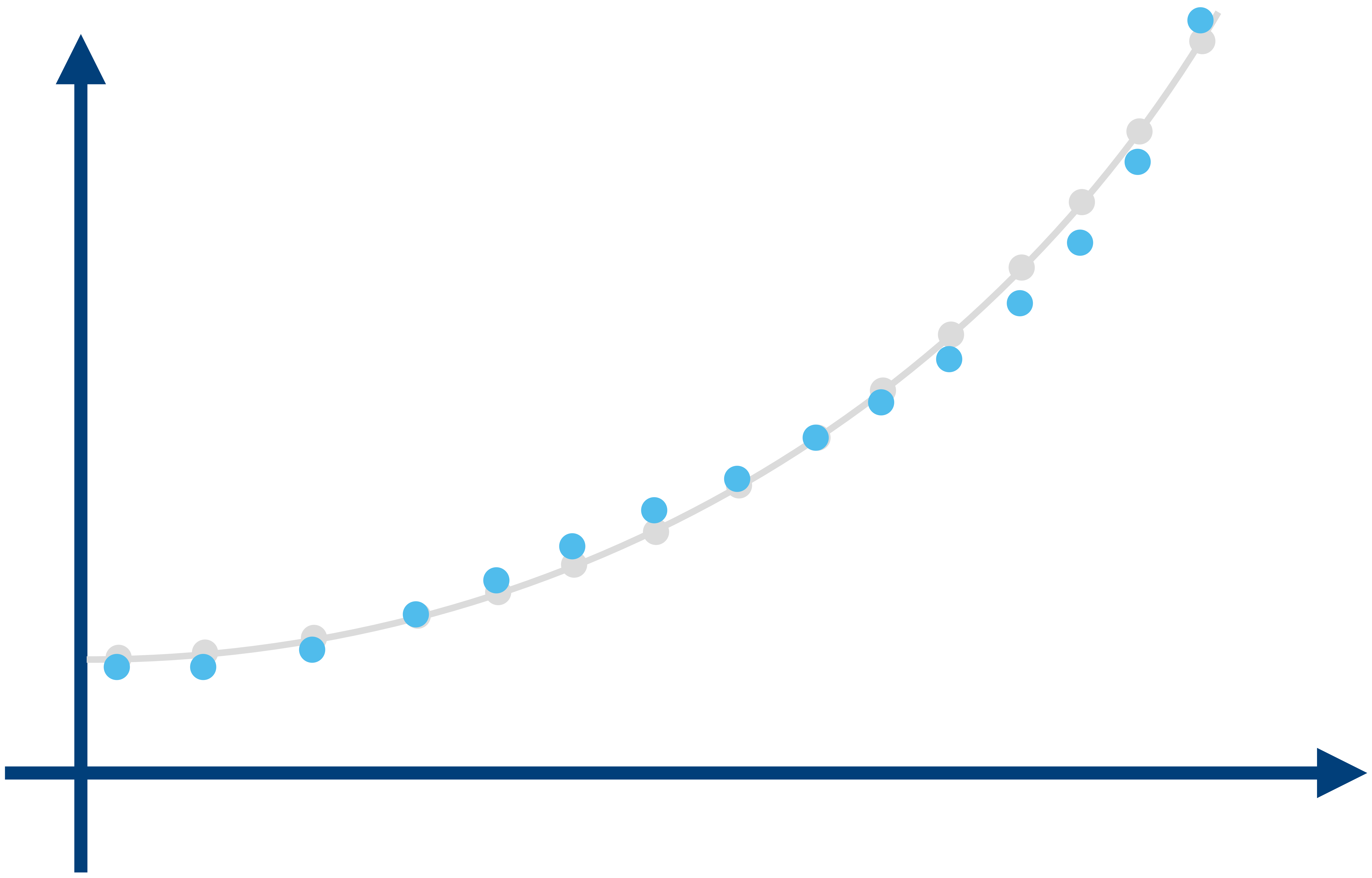


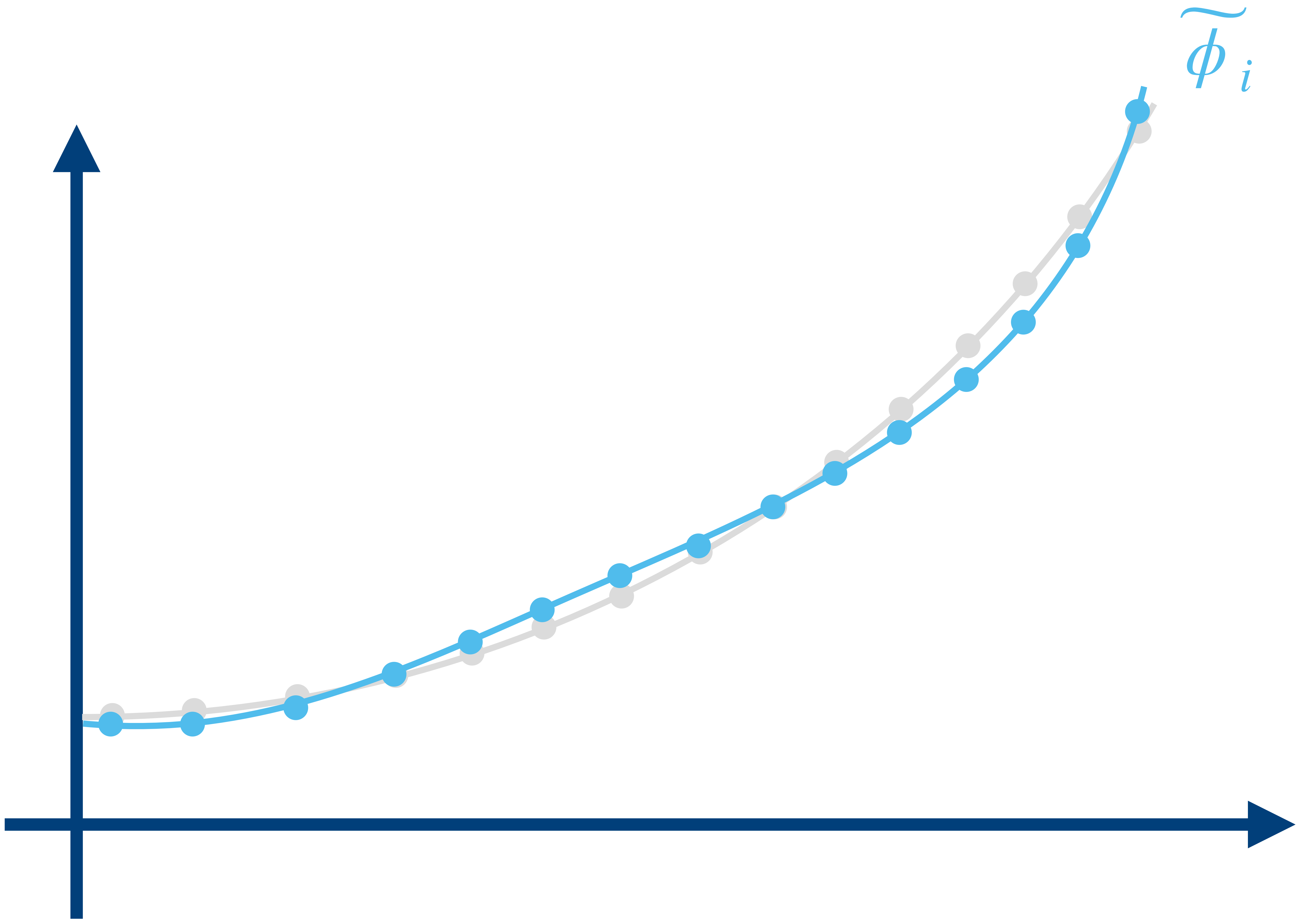
ϕ_i



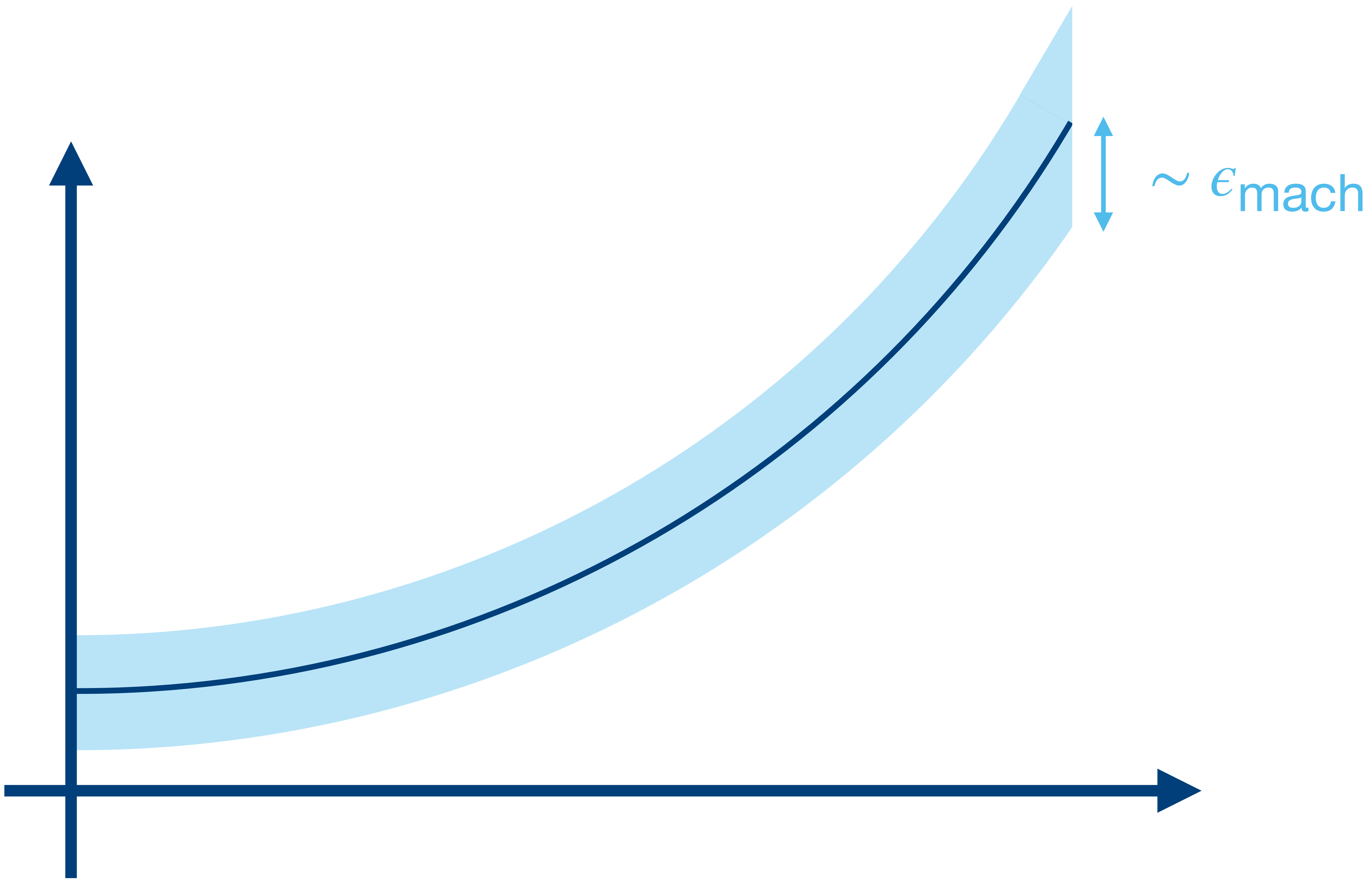



$\widetilde{\phi}_i$

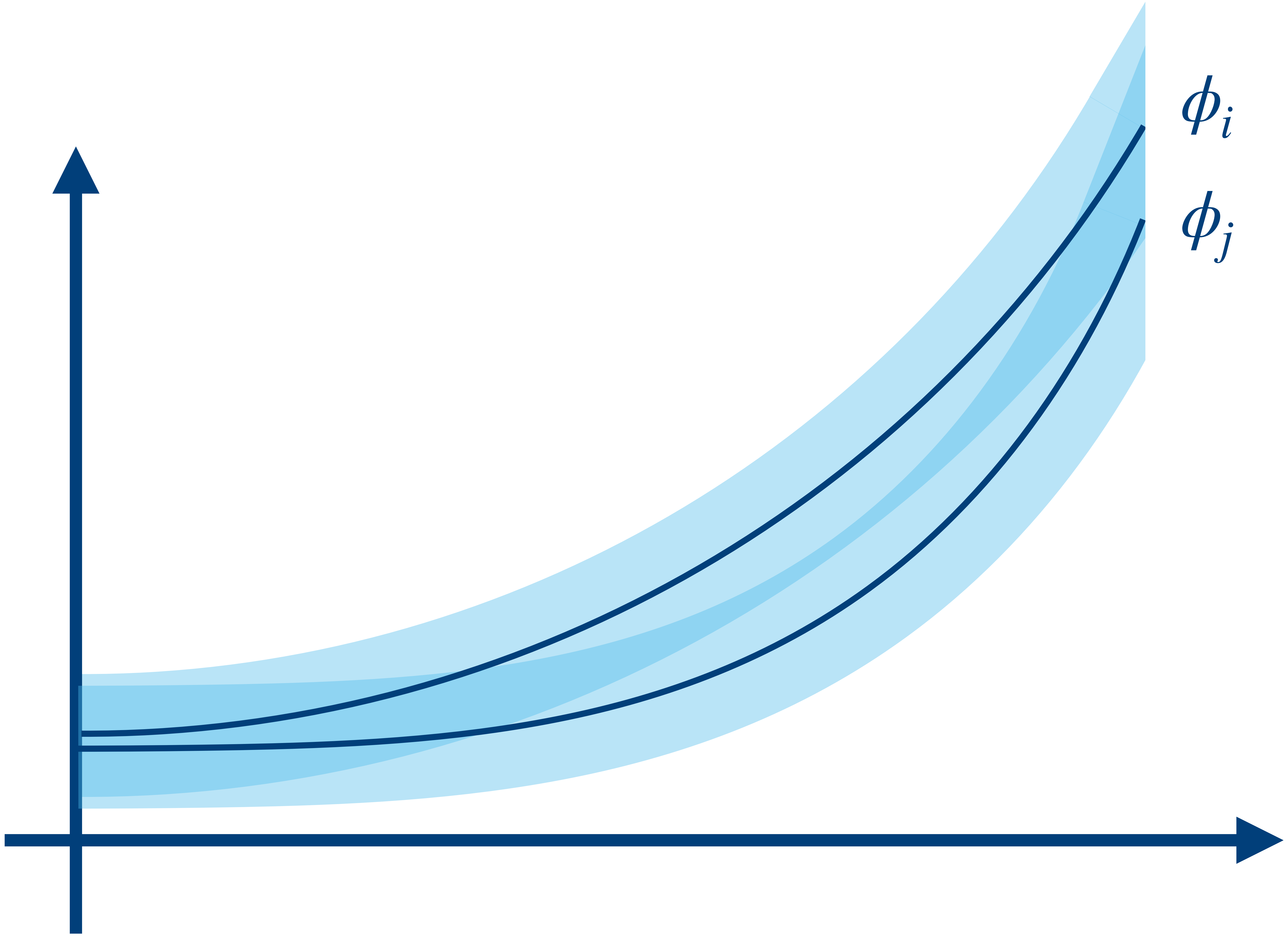




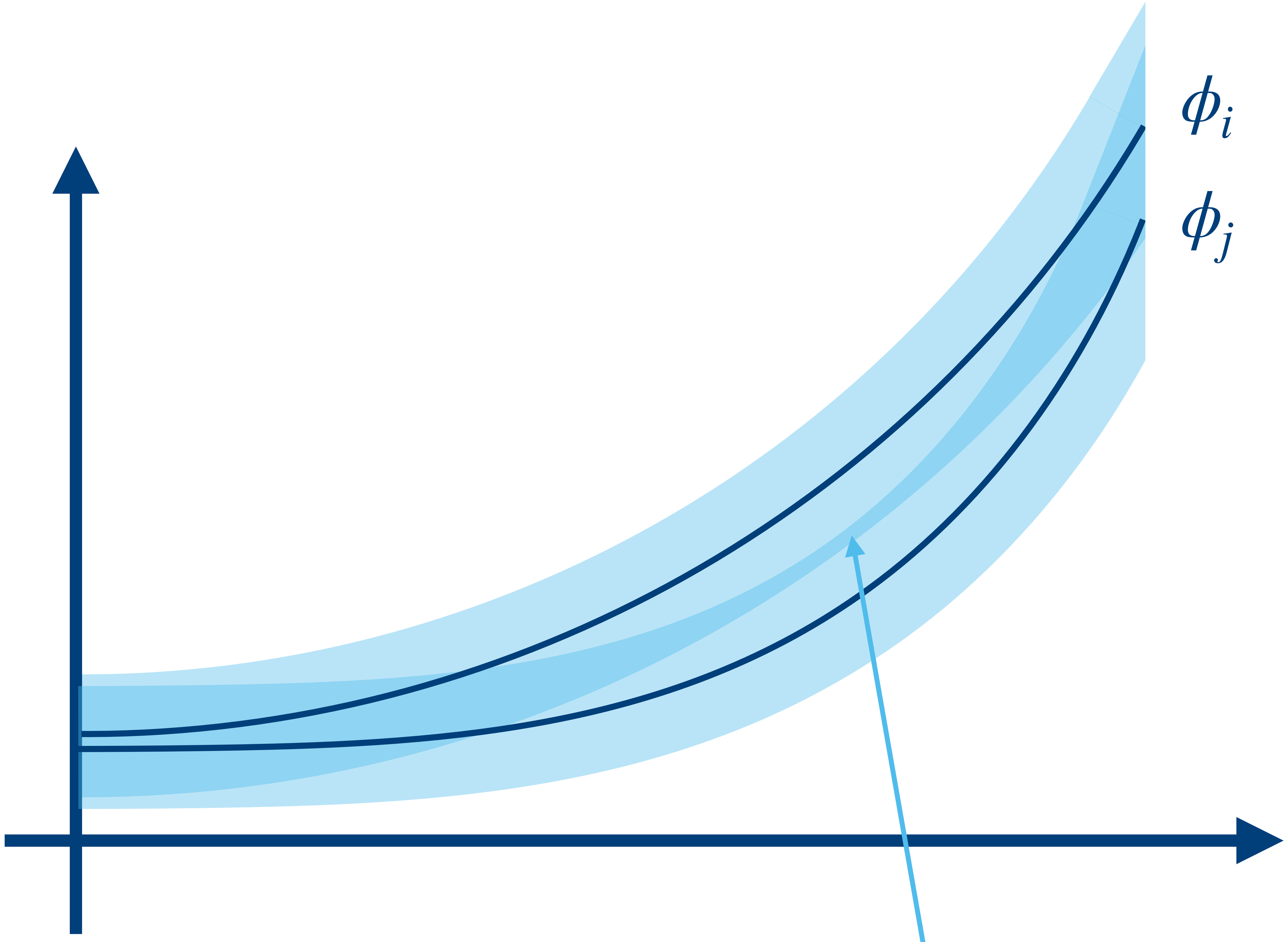
$\widetilde{\phi}_i$



$\sim \epsilon_{\mathrm{mach}}$



ϕ_i
ϕ_j



ϕ_i and ϕ_j are indistinguishable from a numerical point of view

Numerically redundant sets

span a lower dimensional space when analysed numerically rather than analytically

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span a lower dimensional space when analysed numerically rather than analytically

This is equivalent to: the singular values of the synthesis operator

$$\mathcal{T}_n : \mathbb{C}^n \to H, \quad c \mapsto \sum_{i=1}^{n} c_i \phi_i$$

satisfy $\sigma_{\min} \leq \epsilon_{mach} \sigma_{\max}$

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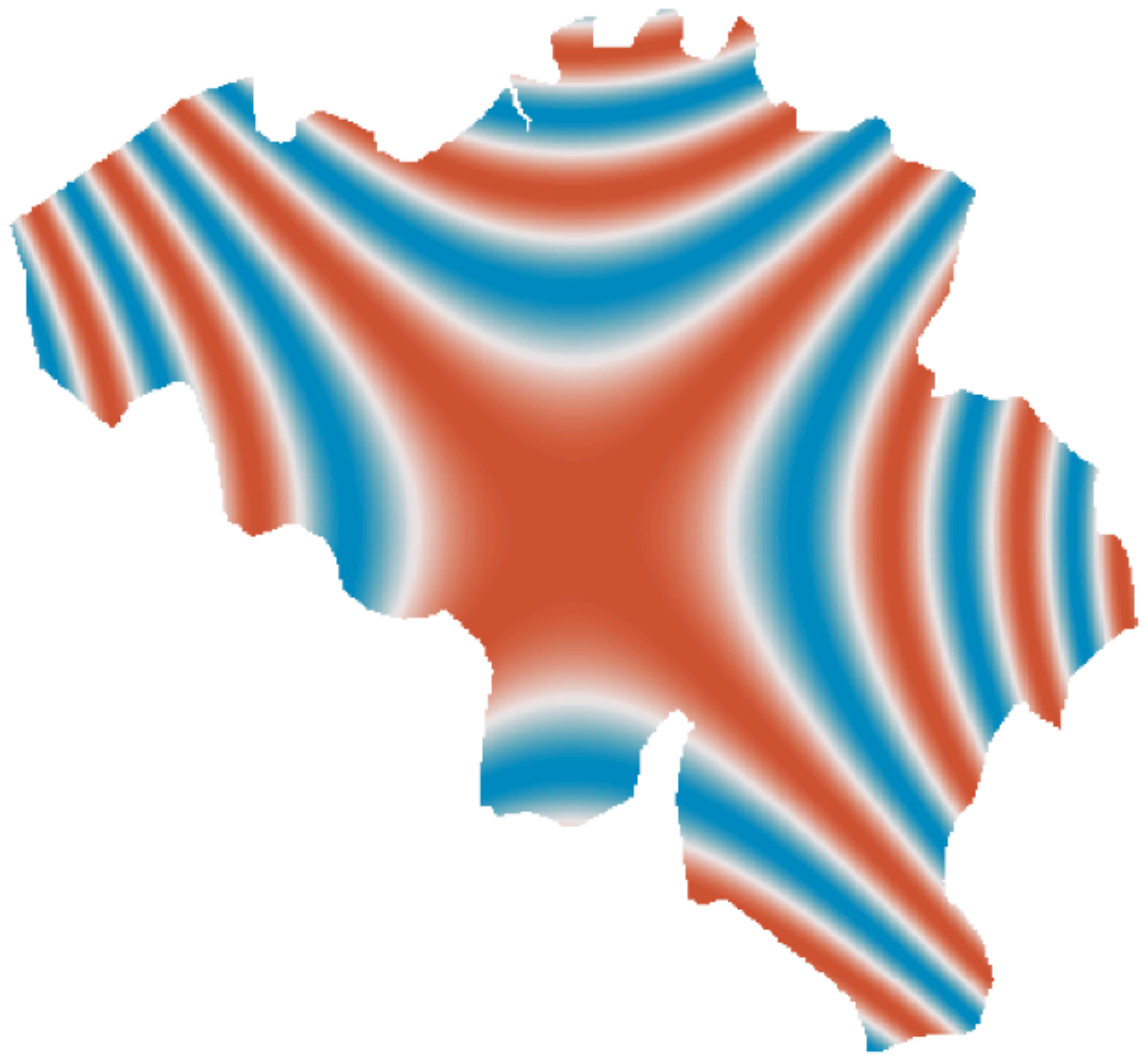
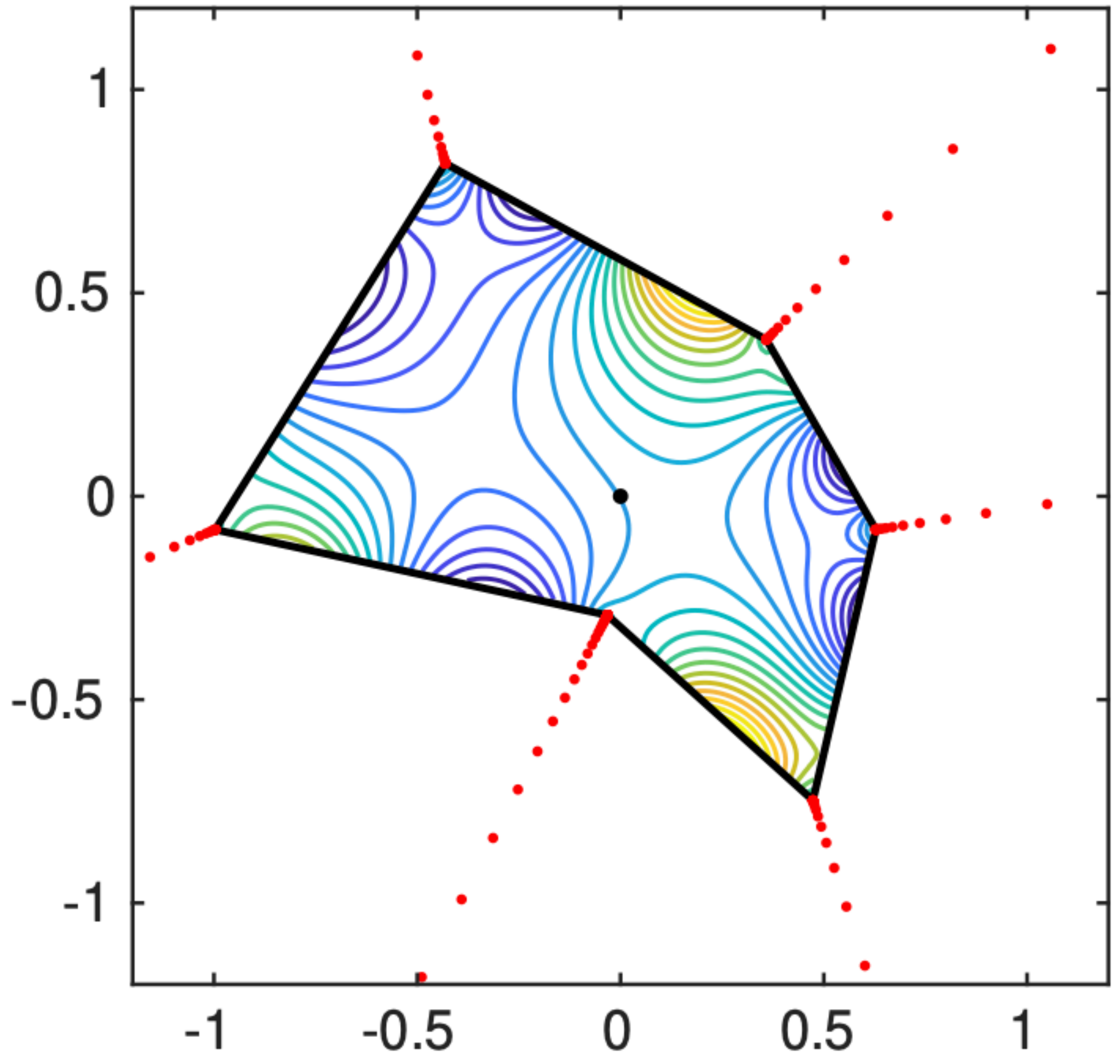
You recognise this if: you have plenty of data on f yet the system of equations to compute coefficients c is ill-conditioned anyway

Numerically redundant sets

offer a lot of flexibility



approximate on irregular domains



incorporate knowledge on f
by combining / weighting bases

left: (Matthysen and Huybrechs, 2018) , right: (Gopal and Trefethen, 2019)

- **The bad news** - slower convergence
- **The ugly news** - regularization
- **The good news** - less data

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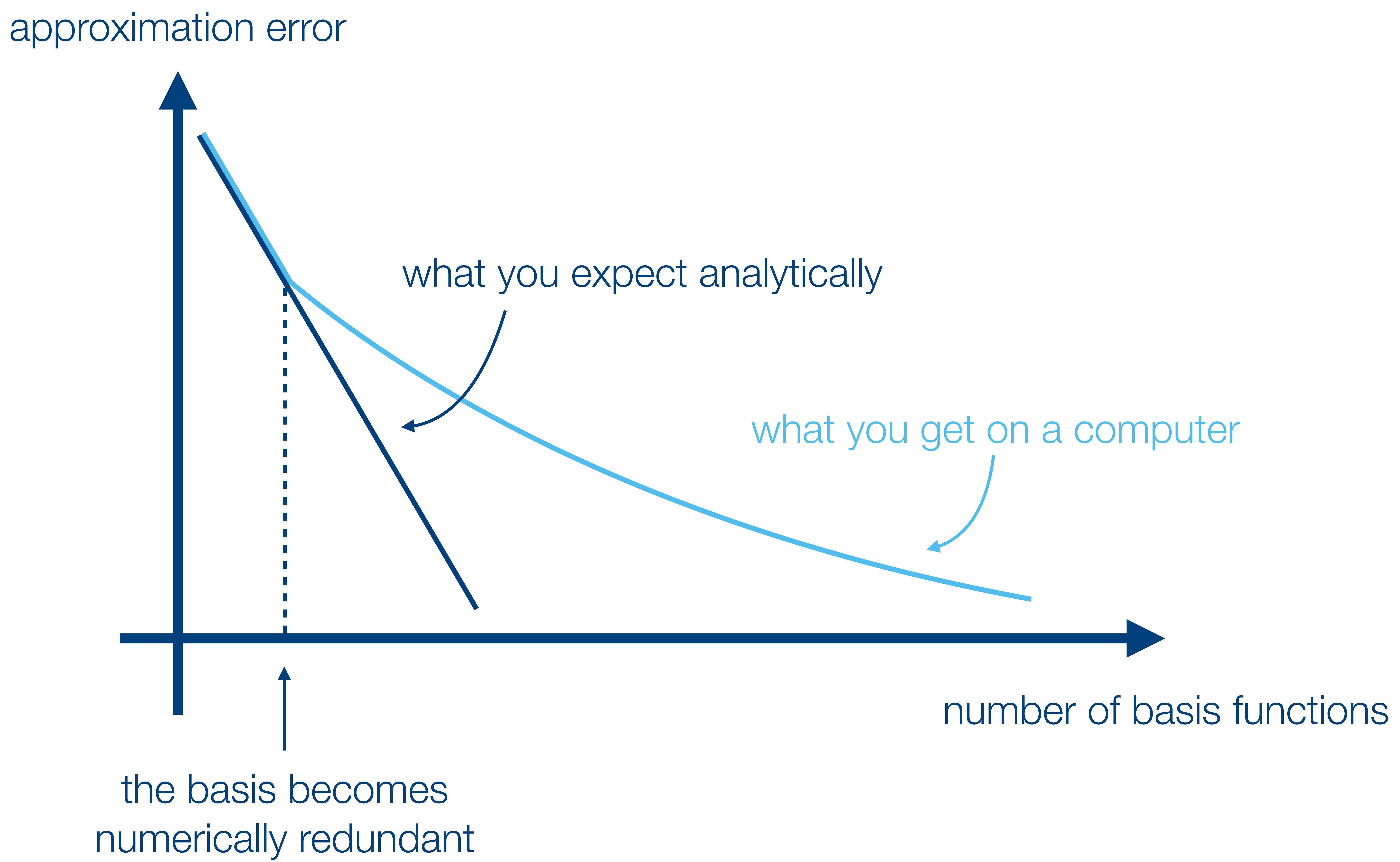
approximation error
what you expect analytically
what you get on a computer
number of basis functions
the basis becomes
numerically redundant

Achievable accuracy

On a computer, the basis functions ϕ_i are perturbed to $\widetilde{\phi}_i$

best approximation error in span(ϕ_i) $\qquad \inf_{c \in \mathbb{C}^n} \left(\|f - \mathcal{T}_n c\| \right)$

best approximation error in span$(\widetilde{\phi}_i)$ $\qquad \leq \inf_{c \in \mathbb{C}^n} \left(\|f - \mathcal{T}_n c\| + \epsilon_{\text{mach}} \|\mathcal{T}_n\| \, \|c\|_2 \right)$

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- the numerical accuracy depends on the norm of the coefficients $\|c\|_2$

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- the numerical accuracy depends on the norm of the coefficients $\|c\|_2$
- the difference is only significant if $\mathcal{T}_n$ has small singular values

Convergence guarantees

Assume $\{\phi_i\}_{i=1}^{n} \subset \{\phi_i\}_{i=1}^{\infty}$ and $f \in \overline{\text{span}}(\{\phi_i\}_{i=1}^{\infty})$, then $f = \sum_{i=1}^{\infty} a_i \phi_i$ and

<u>orthonormal basis</u>	<u>Riesz basis</u>	<u>(overcomplete) frame</u>
a is unique	a is unique	a is not unique
$\|\|a\|\|_2 = \|\|f\|\|$	$A\|\|a\|\|_2^2 \leq \|\|f\|\|^2 \leq B\|\|a\|\|_2^2$	$\exists a : A\|\|a\|\|_2^2 \leq \|\|f\|\| \leq B\|\|a\|\|_2^2$

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subsequence is again an orthonormal / Riesz basis

subsequence is numerically redundant as $n \to \infty$

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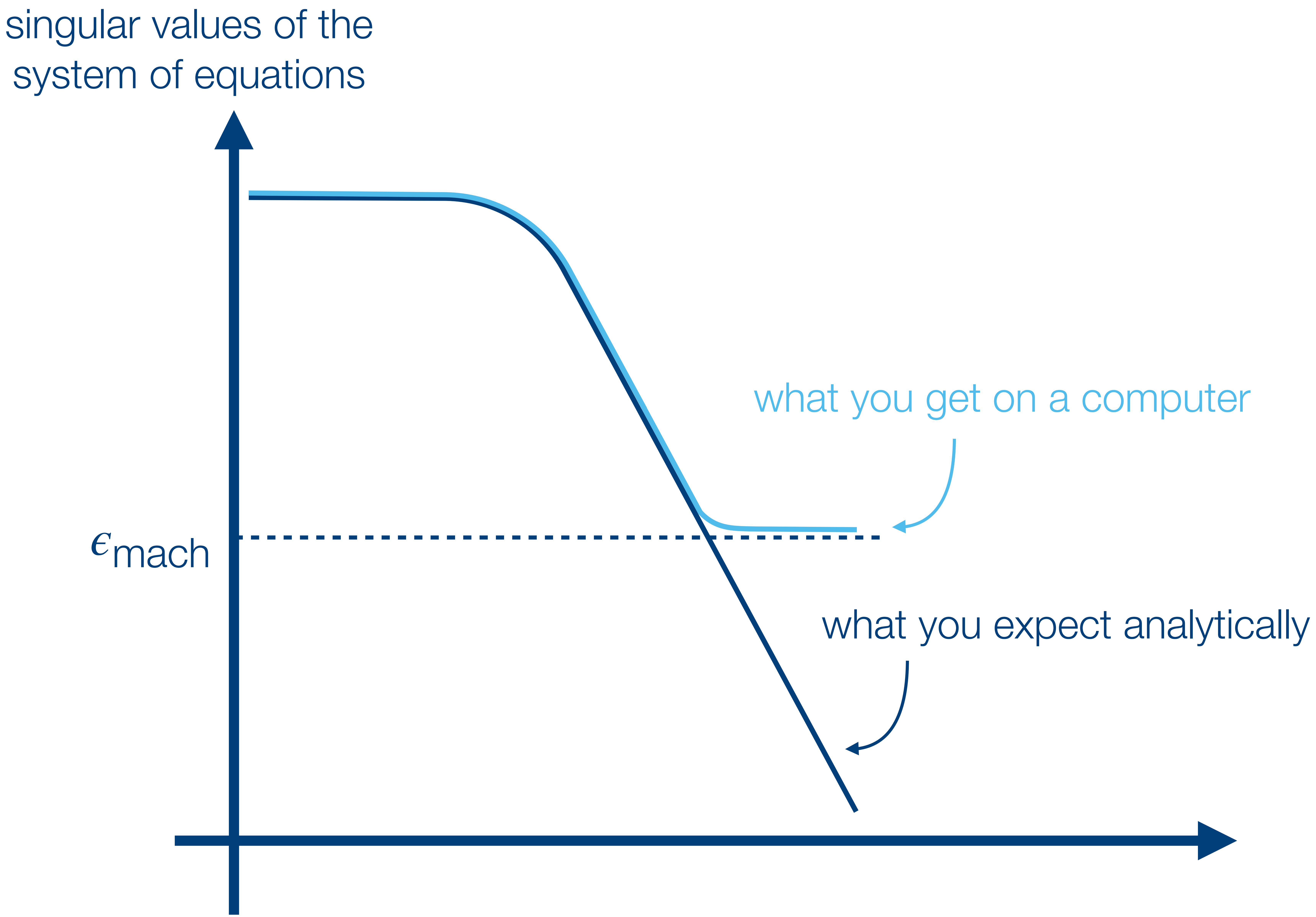
The existence of bounded coefficients $\{a_i\}_{i=1}^{\infty}$ guarantees convergence to ϵ_{mach}

$$\lim_{n\to\infty}\left(\inf_{c\in\mathbb{C}^n}\left(\|f - \mathcal{T}_n c\| + \epsilon_{\text{mach}}\,\|\mathcal{T}_n\|\;\|c\|_2\right)\right) \leq \epsilon_{\text{mach}}\sqrt{\frac{B}{A}}\|f\|$$

- **The bad news** - slower convergence
- **The ugly news** - regularization
- **The good news** - less data


singular values of the system of equations
what you get on a computer
ϵ_{mach}
what you expect analytically

Backward stability

We look for coefficients c that minimize

$$\|Ac - b\|_2 \qquad \text{with } (A)_{i,j} = l_i(\phi_j) \text{ and } (b)_i = l_i(f)$$

where $\{l_i\}_{i=1}^{m}$ are linear sampling functionals

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Numerical algorithms guarantee to compute

$$\hat{c} = \arg\min_c \|(A + \Delta A)c - (b + \Delta b)\|_2 \qquad \text{where } \|\Delta \cdot\|_2 \lesssim \epsilon_{\text{mach}}\|\cdot\|_2$$

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such that

$$\|A\hat{c} - b\|_2 \lesssim \inf_c \|Ac - b\|_2 + \epsilon_{\text{mach}} \left(\|A\|_2 (\|\hat{c}\|_2 + \|c\|_2) + \|b\|_2 \right)$$

Backward stability does not suffice

We look for coefficients c that minimize

$$\|Ac - b\|_2 \qquad \text{with } (A)_{i,j} = l_i(\phi_j) \text{ and } (b)_i = l_i(f)$$

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Numerical algorithms

$$\hat{c} = \arg\min_x \quad \|_2$$

For numerically redundant sets, A is heavily ill-conditioned and $\|\hat{c}\|_2$ can be huge!

such that

$$\|A\hat{c} - b\|_2 \lesssim \inf_c \|Ac - b\|_2 + \epsilon_{\text{mach}} \left(\|A\|_2 (\|\hat{c}\|_2 + \|c\|_2) + \|b\|_2 \right)$$

ℓ^2-regularization

If we penalize the norm of the coefficients

$$\min_c \|Ac - b\|_2^2 + \epsilon^2 \|c\|_2^2 \qquad \text{where } \epsilon \sim \epsilon_{\text{mach}} \|A\|_2$$

then backward stable algorithms guarantee

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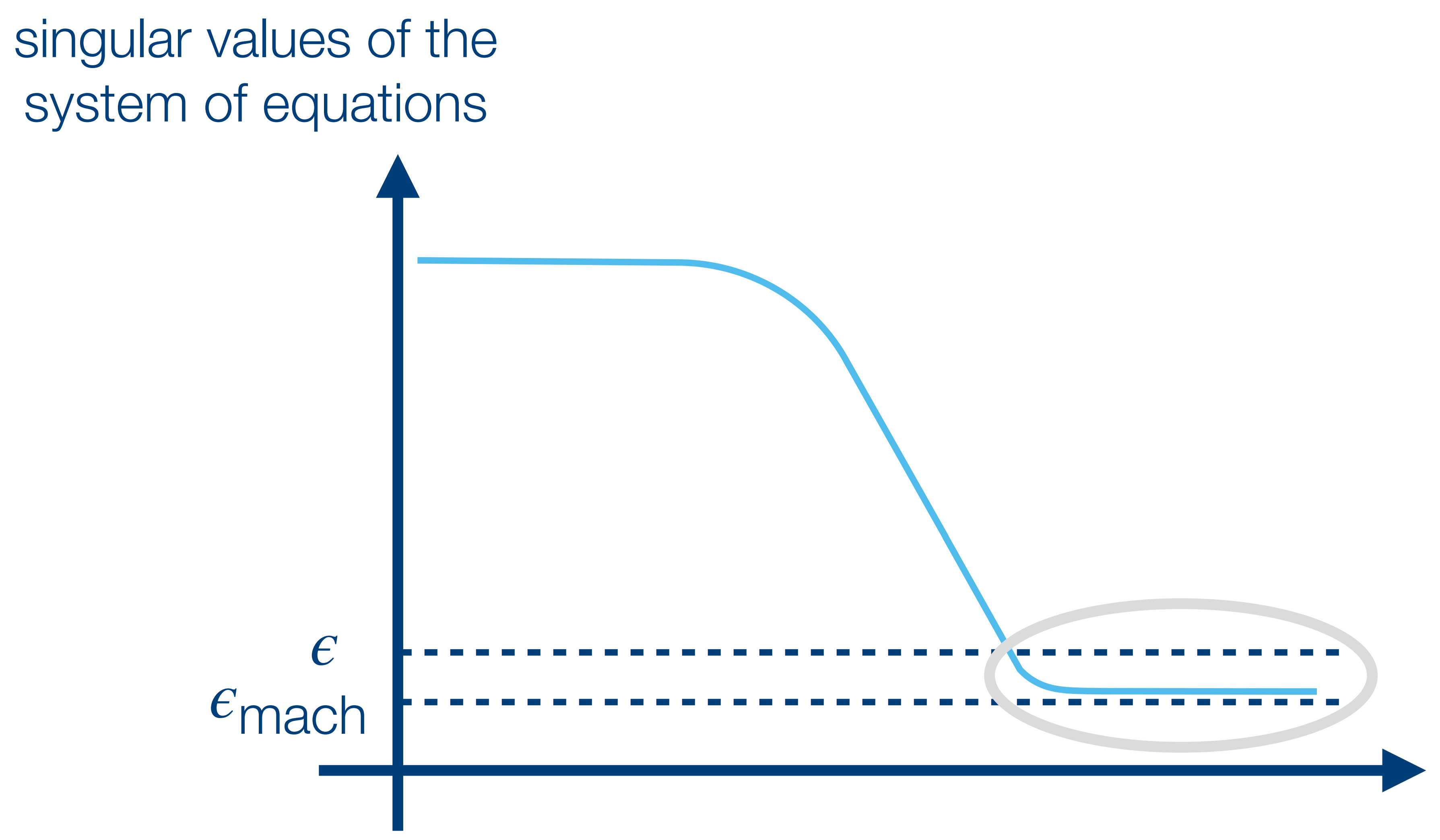
<u>Remember</u>: the numerically achievable accuracy equals

$$\inf_c \left(\|\mathcal{T}_n c - f\| + \epsilon_{\text{mach}} \|\mathcal{T}_n\| \, \|c\|_2 \right)$$

Common strategies

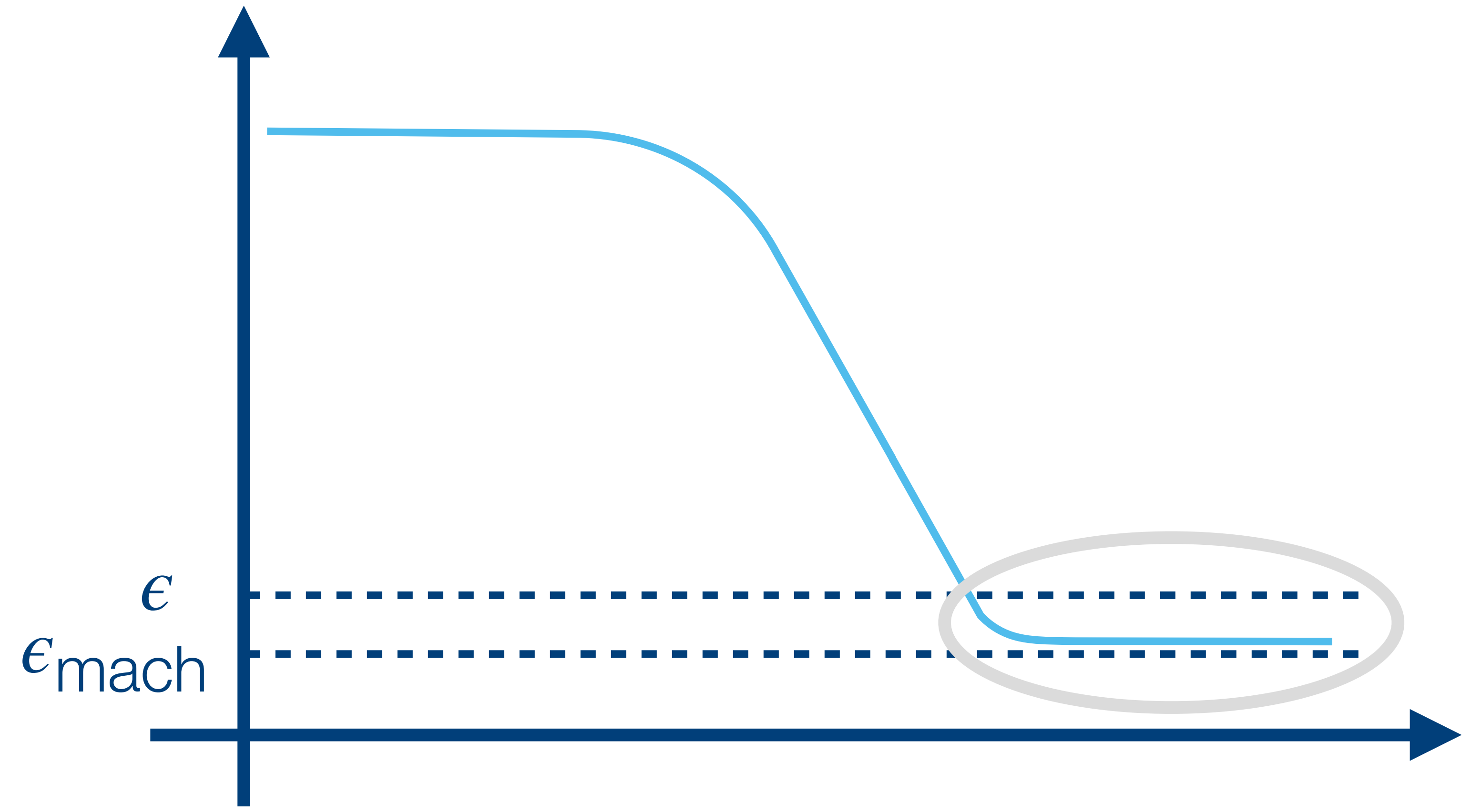
ℓ^2-regularization

- Tikhonov regularization
- truncated singular value decomposition (TSVD)



! standard routines such as Matlab's `backslash` regularize under the hood

Common strategies



ℓ^2-regularization

- Tikhonov regularization
- truncated singular value decomposition (TSVD)

Numerical orthogonalization on a dense grid $\{t_j\}_{j=1}^{m}$

$$(T + \Delta T) = QR$$

where $T = \begin{bmatrix} \phi_1(t_1) & \dots & \phi_n(t_1) \\ \vdots & & \vdots \\ \phi_1(t_m) & \dots & \phi_n(t_m) \end{bmatrix}$ and $\|\Delta T\| \lesssim \epsilon_{\text{mach}} \|T\|_2$

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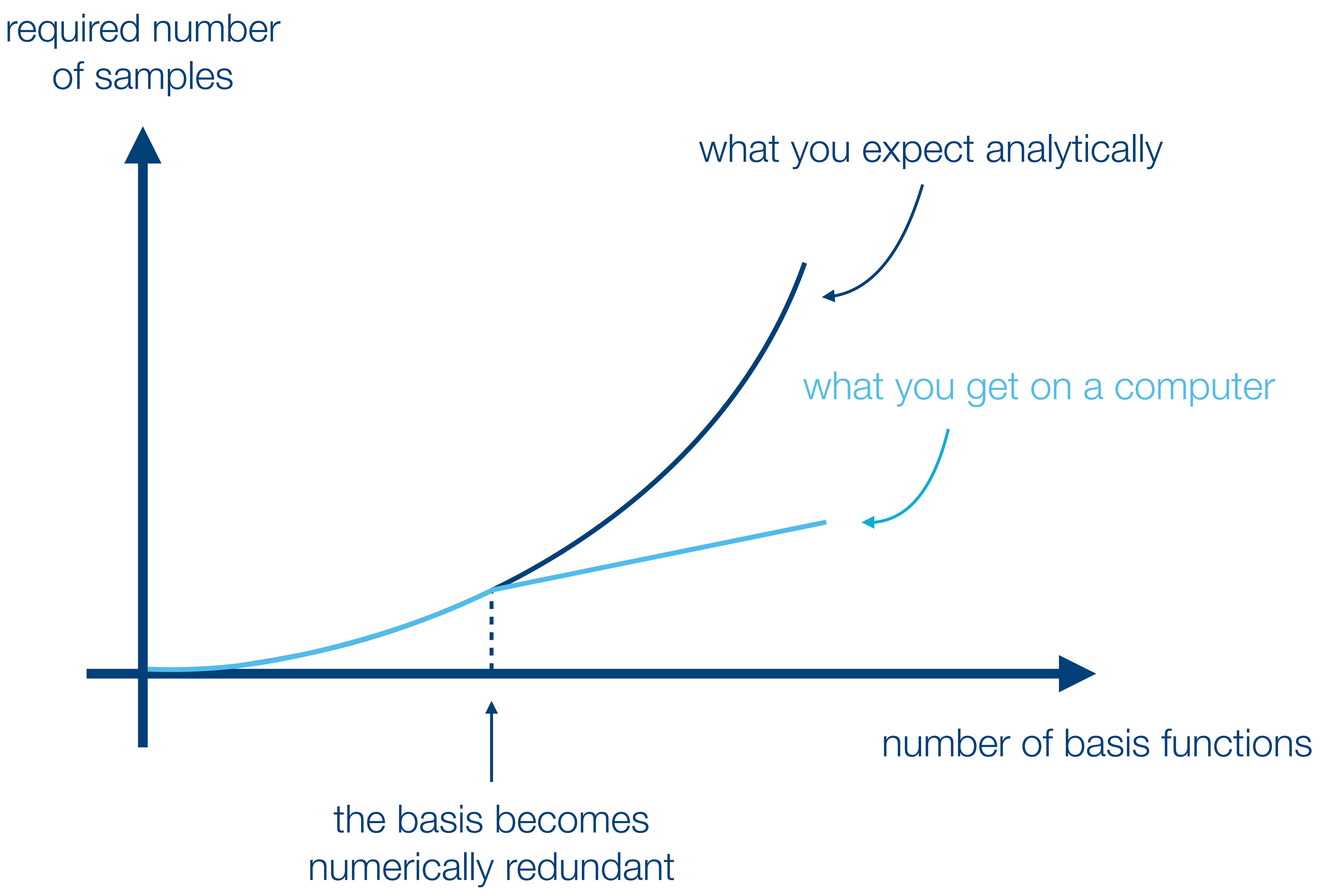
required number
of samples
what you expect analytically
what you get on a computer
number of basis functions
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Error analysis

We discretize using the sampling operator $\mathscr{M}_m : f \mapsto \{l_j(f)\}_{j=1}^m$ defining $\|\cdot\|_m = \|\mathscr{M}_m \cdot\|_2$

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Analytical behaviour

$$c = \arg\min_x \|\mathscr{T}_n x - f\|_m^2$$

then we obtain

$$\|\mathscr{T}_n c - f\| \leq \left(1 + \frac{\|\mathscr{M}_m\|}{\sqrt{A_{n,m}}}\right) \inf_x \|\mathscr{T}_n x - f\|$$

where

$$A_{n,m}\|v\|^2 \leq \|v\|_m^2, \quad \forall v \in \text{span}(\{\phi_i\}_i)$$

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Numerical behaviour

$$c = \arg\min_x \|\mathscr{T}_n x - f\|_m^2 + \epsilon^2 \|x\|_2^2$$

then if

$$\|\mathscr{T}_n c - f\| \leq \left(1 + \frac{\|\mathscr{M}_m\|}{\sqrt{A_{n,m}^\epsilon}}\right) \inf_x \|\mathscr{T}_n x - f\| + \epsilon\|x\|_2$$

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$$A_{n,m}^\epsilon \|\mathscr{T}_n x\|^2 \leq \|\mathscr{T}_n x\|_m^2 + \epsilon^2 \|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

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Numerical behaviour

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then if

$$\|\mathscr{T}_n c - f\| \leq \left(1 + \frac{\|\mathscr{M}_m\|}{\sqrt{A^\epsilon_{n,m}}}\right) \inf_x \|\mathscr{T}_n x - f\| + \epsilon\|x\|_2$$

where

$$A^\epsilon_{n,m}\|\mathscr{T}_n x\|^2 \leq \|\mathscr{T}_n x\|_m^2 + \epsilon^2\|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

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$$A_{n,m}^\epsilon\|\mathscr{T}_n x\|^2 \leq \|\mathscr{T}_n x\|_m^2 + \epsilon^2\|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

Discretization condition

Analytical behaviour

$$A_{n,m}\|v\|^2 \leq \|v\|_m^2, \quad \forall v \in \mathrm{span}(\{\phi_i\}_i)$$

$$\Leftrightarrow A_{n,m}G_n \preceq G_{n,m}$$

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$(G_n)_{i,j} = \langle \phi_i, \phi_j \rangle$ and $(G_{n,m})_{i,j} = \langle \mathcal{M}_m\phi_i, \mathcal{M}_m\phi_j \rangle_2$

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- Independent of the spanning set $\{\phi_i\}_i$: we can use an ONB for the analysis s.t. $G_n = I$

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Numerical behaviour

$$A_{n,m}^{\epsilon}\|\mathcal{T}_n x\|^2 \leq \|\mathcal{T}_n x\|_m^2 + \epsilon^2\|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

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- Dependent on the spanning set $\{\phi_i\}_i$

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- Dependent on the spanning set $\{\phi_i\}_i$

How do we find sampling functionals that satisfy these norm inequalities?

Christoffel sampling

Analytical behaviour

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Numerical behaviour

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$A_{n,m}$ close to 1 w.h.p. when using

$$m \geq Cn \log(n)$$

pointwise random samples with probability depending on

$$k_n(x) = \sum_{i=1}^{n} |u_i(x)|^2$$

Numerical behaviour

$$A_{n,m}^{\epsilon}\|\mathcal{T}_n x\|^2 \leq \|\mathcal{T}_n x\|_m^2 + \epsilon^2\|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

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the inverse Christoffel function / continuous analogue of leverage scores

Numerical behaviour

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$A_{n,m}^{\epsilon}$ close to 1 w.h.p. when using

$$m \ge Cn^{\epsilon}\log(n^{\epsilon})$$

pointwise random samples with probability depending on

$$k_n^{\epsilon}(x) = \sum_{i=1}^n \frac{\sigma_i^2}{\sigma_i^2 + \epsilon^2}|u_i(x)|^2$$

Christoffel sampling

Analytical behaviour

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Numerical behaviour

$$A_{n,m}^{\epsilon}\|\mathcal{T}_n x\|^2 \leq \|\mathcal{T}_n x\|_m^2 + \epsilon^2\|x\|_2^2, \quad \forall x \in \mathbb{C}^n$$

$$\Leftrightarrow A_{n,m}^{\epsilon} G_n \preceq G_{n,m} + \epsilon^2 I$$

effective dimension

$$n^{\epsilon} = \sum_{i=1}^{n} \frac{\sigma_i^2}{\sigma_i^2 + \epsilon^2}$$

$A_{n,m}^{\epsilon}$ close to 1 w.h.p. when using

$$m \geq Cn^{\epsilon}\log(n^{\epsilon})$$

pointwise random samples with probability depending on

$$k_n^{\epsilon}(x) = \sum_{i=1}^{n} \frac{\sigma_i^2}{\sigma_i^2 + \epsilon^2}|u_i(x)|^2$$

Christoffel sampling

Analytical behaviour

$$A_{n,m}\|v\|^2 \leq \|v\|_m^2, \quad \forall v \in \mathrm{span}(\{\phi_i\}_i)$$

$$\Leftrightarrow A_{n,m} I \preceq G_{n,m}^{ONB}$$

$A_{n,m}$ close to 1 w.h.p. when using

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$$k_n(x) = \sum_{i=1}^{n} |u_i(x)|^2$$

Numerical behaviour

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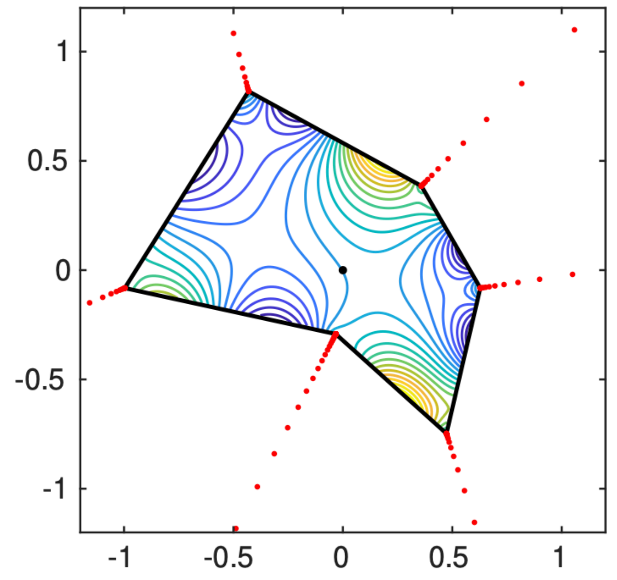
continuous analogue of ridge leverage scores

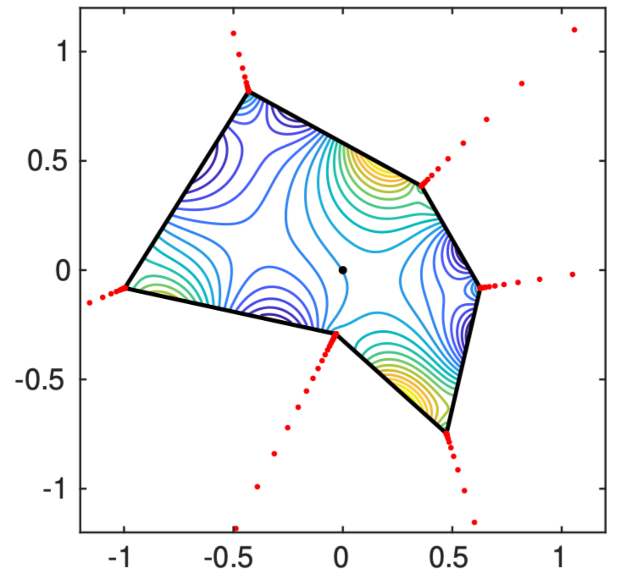
Deterministic sampling



Approximation of $f(x) = J_{1/2}(x+1) + \dfrac{1}{x^2+1}$ on [-1,1] using the basis

$$\{p_i(x)\}_{i=1}^{40} \cup \{w(x)\, p_i(x)\}_{i=1}^{40} \qquad \text{with } w(x) = \sqrt{x+1}$$

Deterministic sampling



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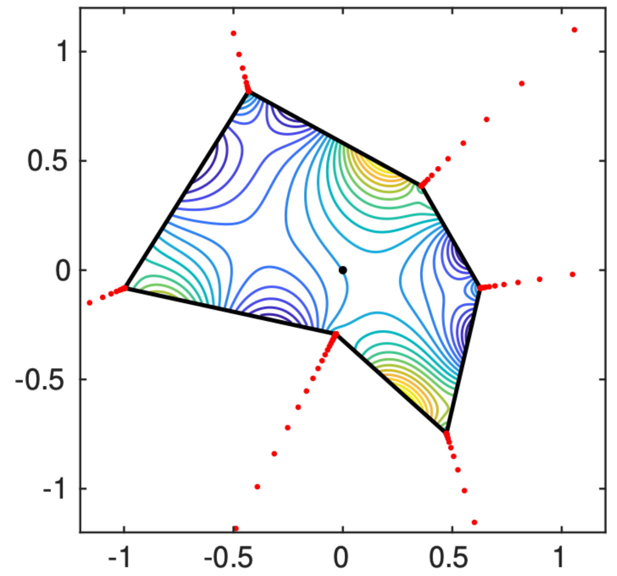

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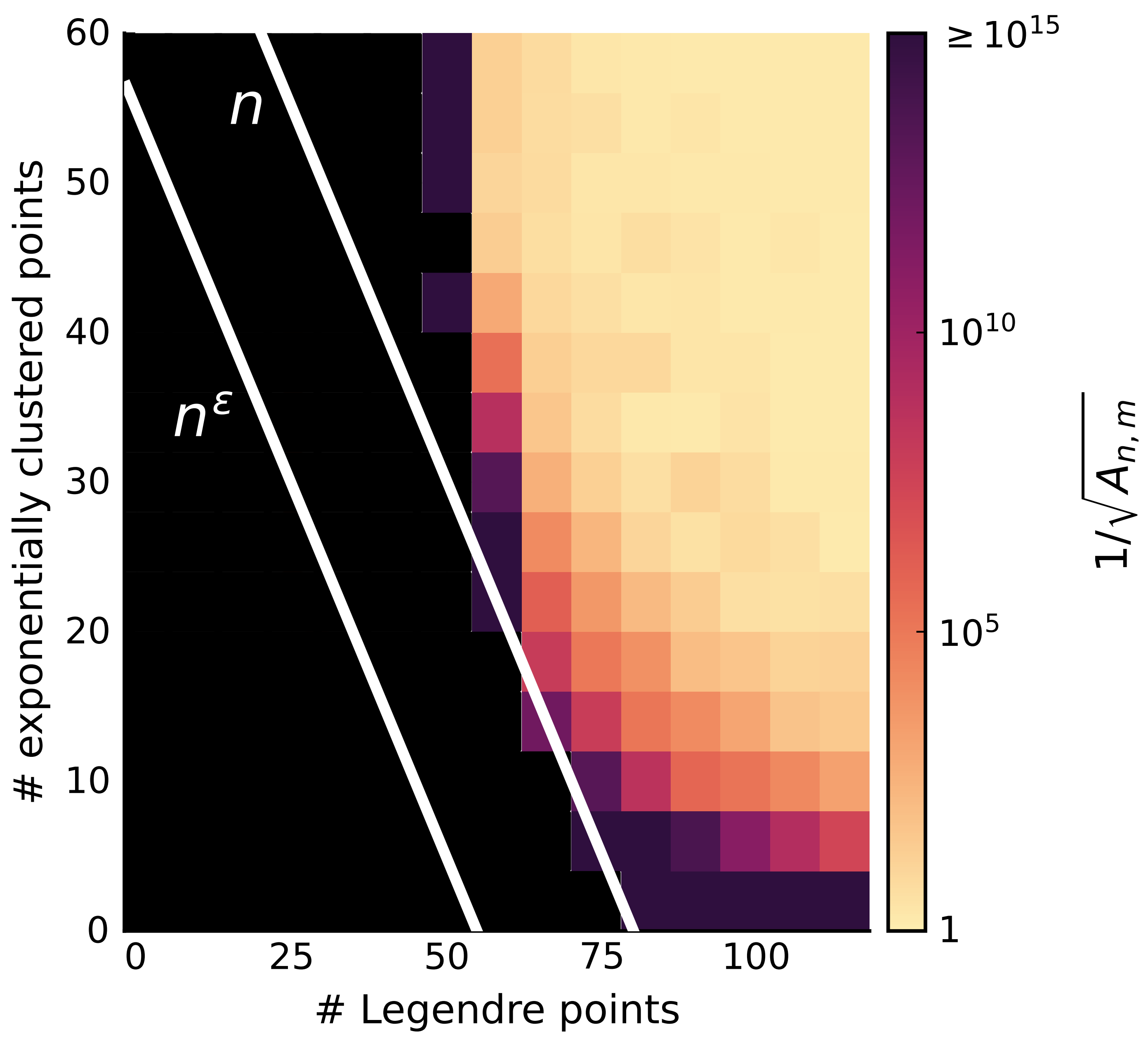
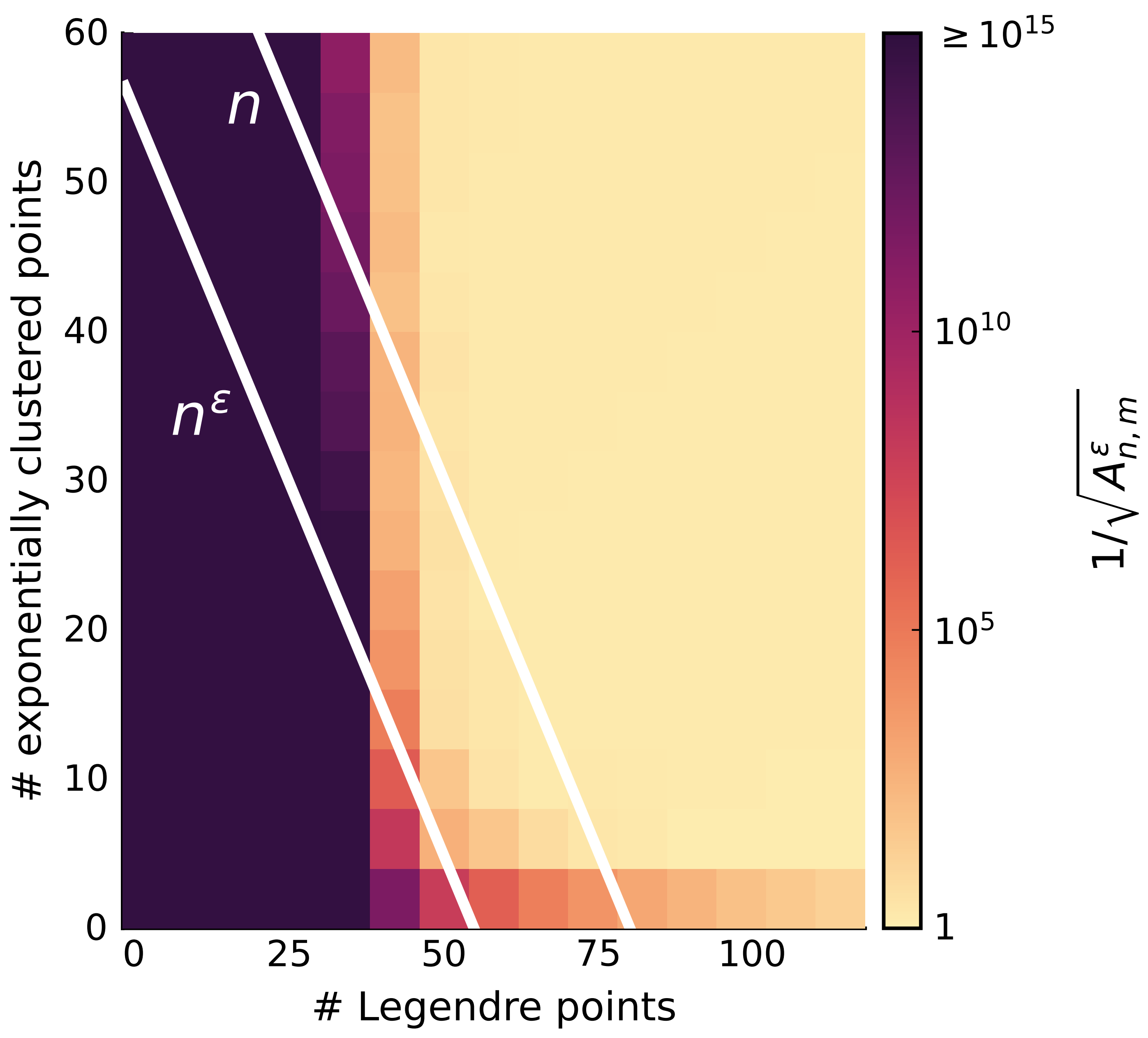
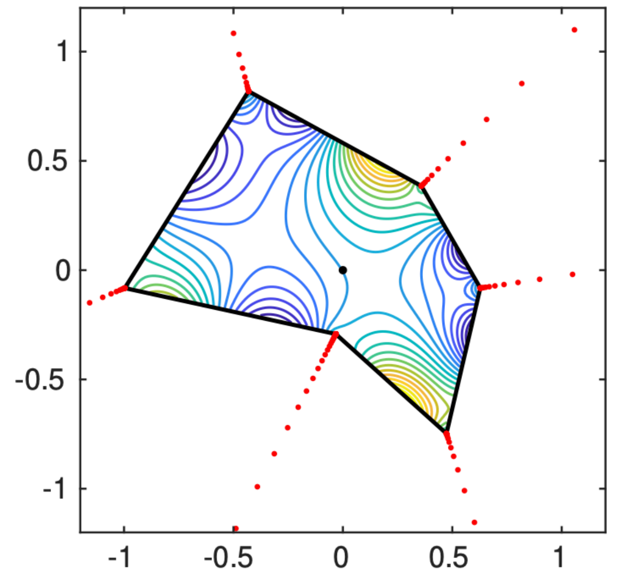
analytical analysis



numerical analysis



Deterministic sampling



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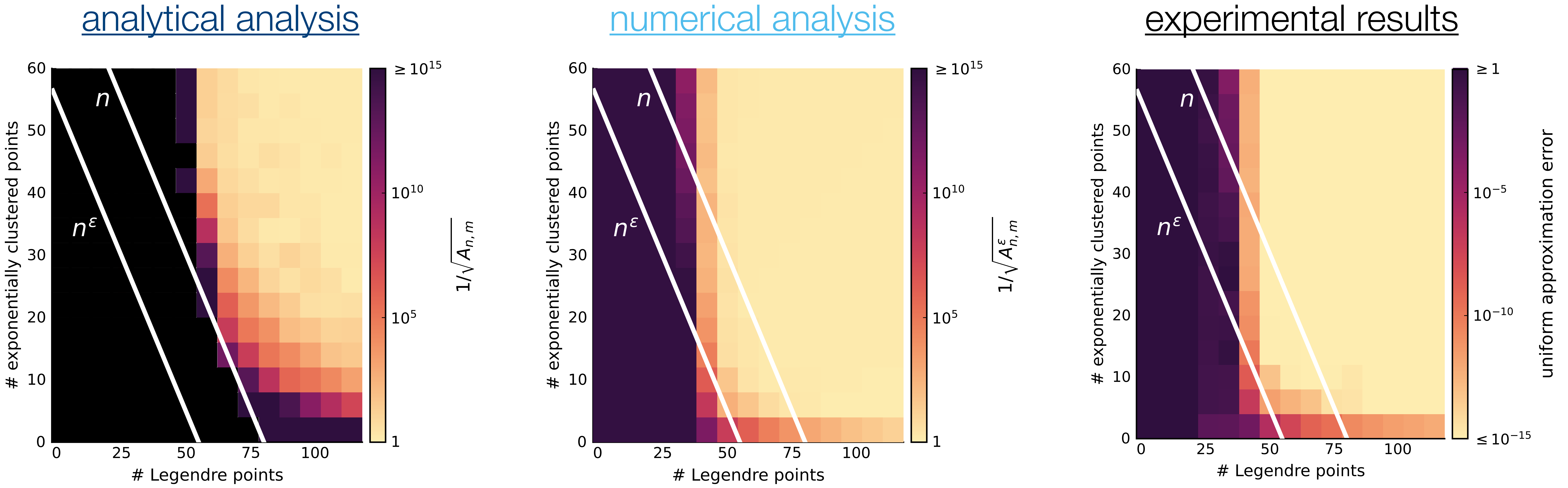

Random sampling

Approximation on $[-0.3, 0.3]$ using a Fourier extension on $[-0.5, 0.5]$

$$\phi_k = \exp(2\pi i x k), \qquad -(n-1)/2 \le k \le (n-1)/2$$

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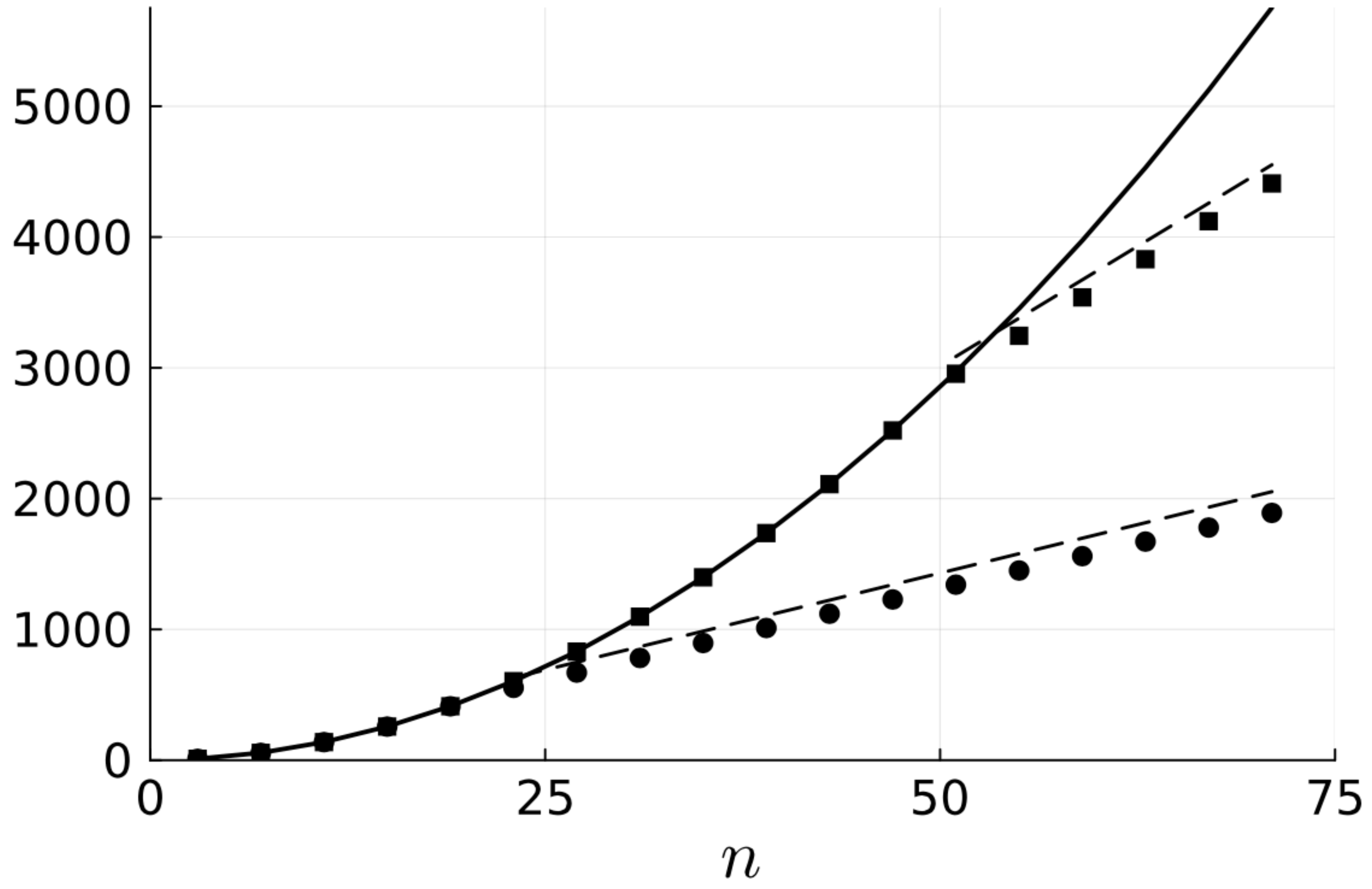
When using <u>uniformly random</u> samples, the required number of samples equals

$$m \geq C\|k_n\|_\infty \log(n) \qquad \text{vs} \qquad m \geq C\|k_n^\epsilon\|_\infty \log(n^\epsilon)$$

(analytically) (numerically)

Random sampling

$m \geq C\|k_n\|_\infty \log(n)$ (analytically) vs $m \geq C\|k_n^\epsilon\|_\infty \log(n^\epsilon)$ (numerically)



$\|k_n\|_\infty = \mathcal{O}(n^2)$

$\|k_n^\epsilon\|_\infty = \mathcal{O}(n)$ (double precision)

$\|k_n^\epsilon\|_\infty = \mathcal{O}(n)$ (single precision)

Conclusions

- **The bad news** - slower convergence
- **The ugly news** - regularization
- **The good news** - less data

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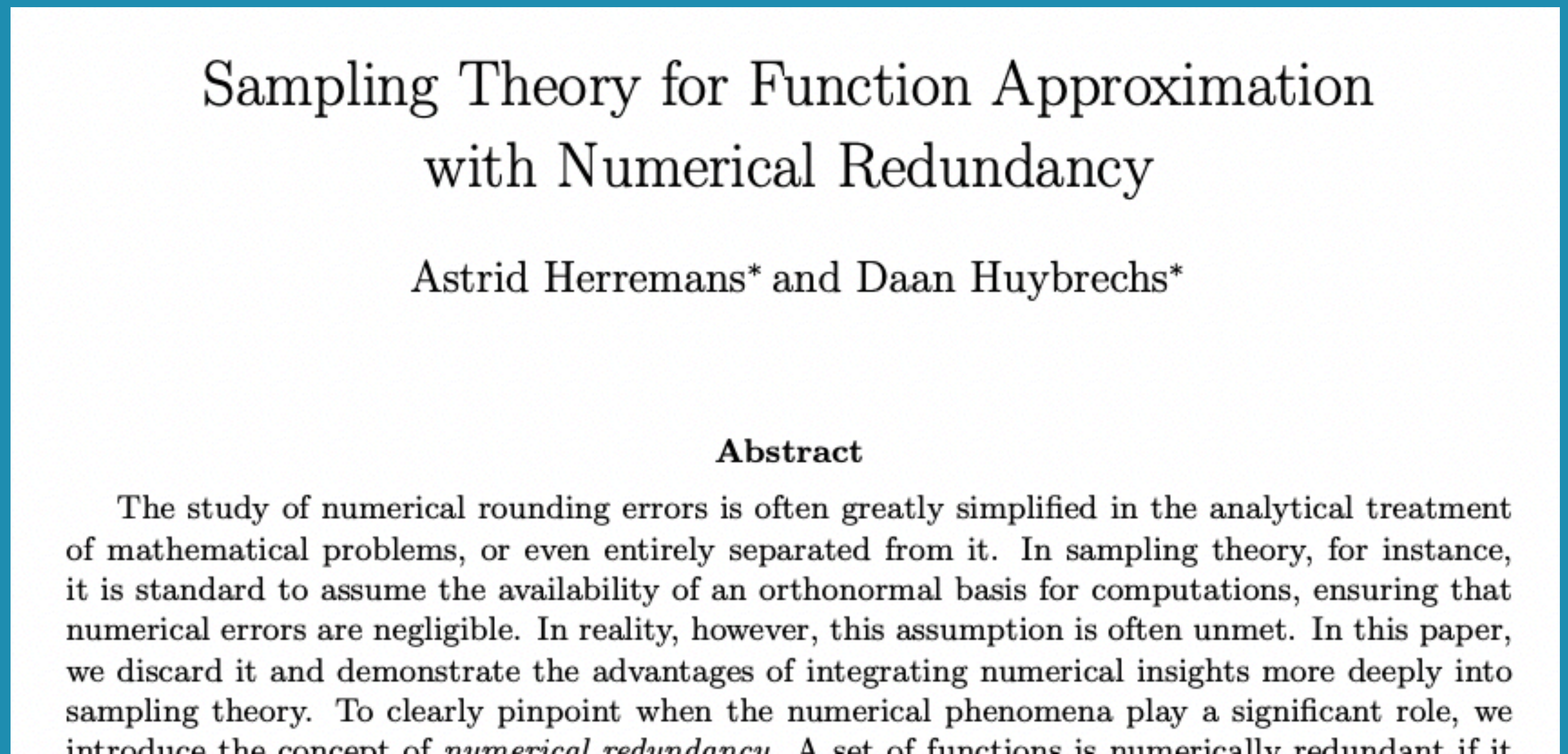
Sampling Theory for Function Approximation with Numerical Redundancy

Astrid Herremans* and Daan Huybrechts*

Abstract

The study of numerical rounding errors is often greatly simplified in the analytical treatment of mathematical problems, or even entirely separated from it. In sampling theory, for instance, it is standard to assume the availability of an orthonormal basis for computations, ensuring that numerical errors are negligible. In reality, however, this assumption is often unmet. In this paper, we discard it and demonstrate the advantages of integrating numerical insights more deeply into sampling theory. To clearly pinpoint when the numerical phenomena play a significant role, we

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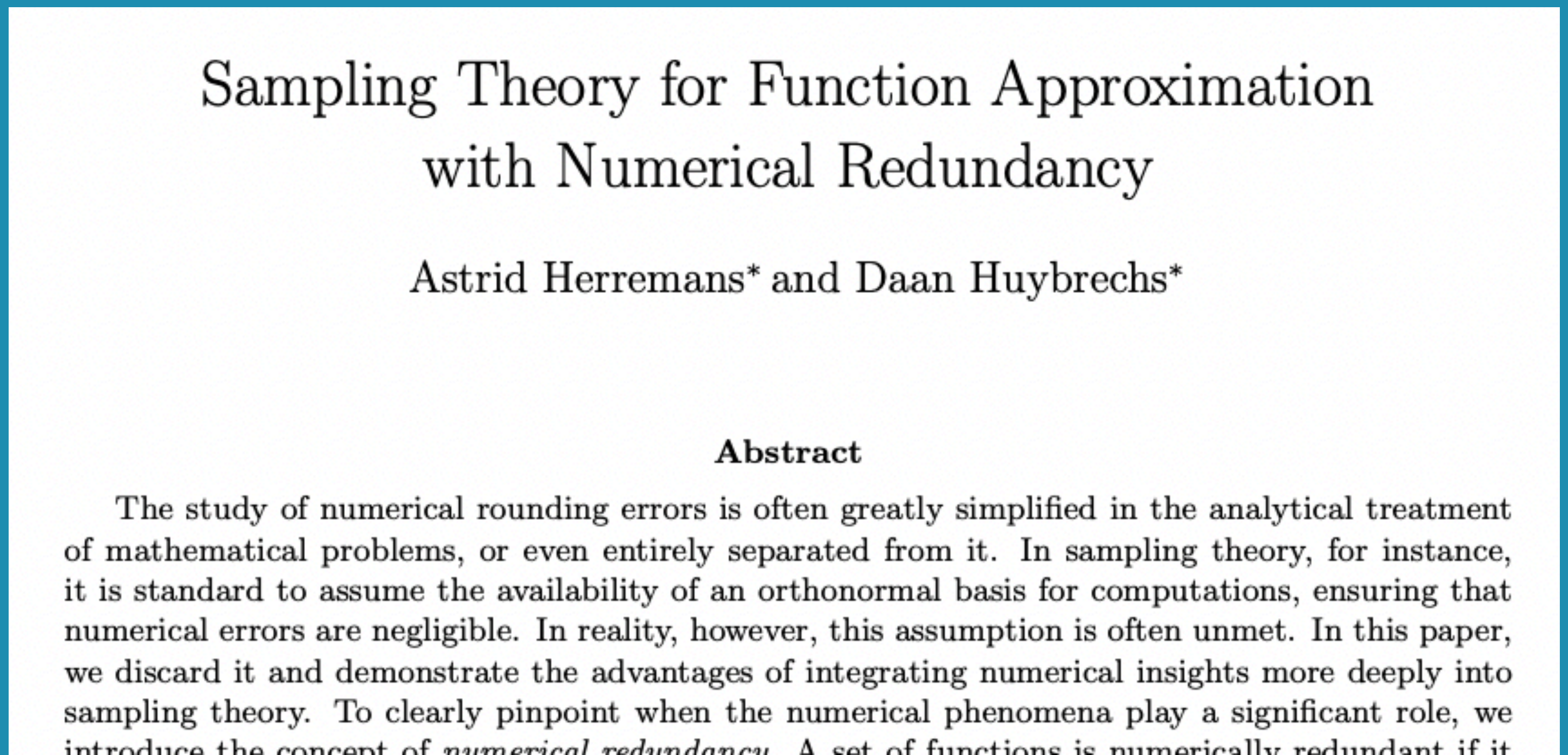
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