

GOODE: A GAUSSIAN OFF-THE-SHELF ORDINARY DIFFERENTIAL EQUATION SOLVER

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GOODE: A Gaussian Off-The-Shelf ODE Solver

What are we doing?

Ordinary Differential Equations (ODEs)

$$\frac{d}{dt} \mathbf{y}(t) = \mathbf{f}(\mathbf{y}(t), t)$$

Vector-valued, changes in time

- ▶ Important mathematical models
- ▶ Broad range of applications

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- ▶ Important mathematical models
- ▶ Broad range of applications
- ▶ Recently ODE (solver) also in ML, e.g.
 - ▶ Building blocks in NNets [Chen 2018] Neural ODEs
 - ▶ [Grathwohl 2019] FFJORD
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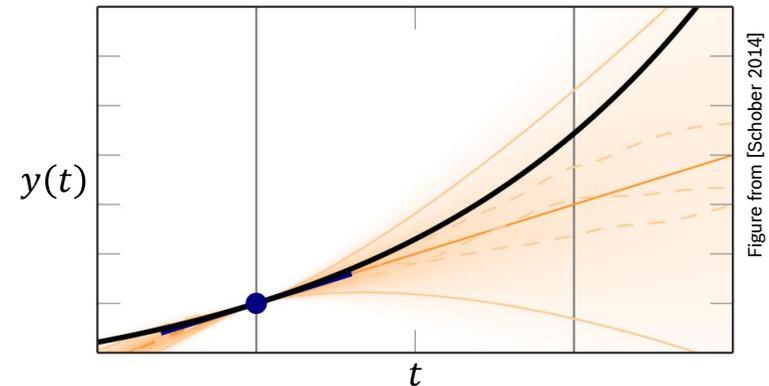
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ODE approximation! → Error!

Probabilistic Numerical Methods (PNMs)

- ▶ Return probability distributions
- ▶ Represent numerical approximation error



Be certain about your uncertainty!

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More specific!

What is the problem?

Nonlinear two-point
Boundary Value Problem (BVP)

Find $y: [a, b] \rightarrow \mathbb{R}^d$ such that

$$\text{ODE} \quad y'(t) = f(y(t), t)$$

$$\text{BC} \quad \mathbf{0} = g(y(a), y(b))$$

Standard non-probabilistic solver exist.

But no general-purpose probabilistic solver!

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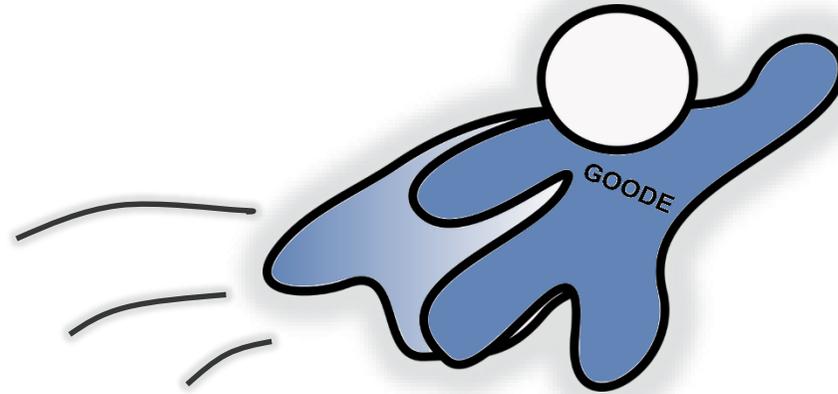
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GOODE specs

- ❖ Novel functionality: probability distribution over solution space
- ❖ Intrinsic error estimation
- ❖ Convergence theory exists

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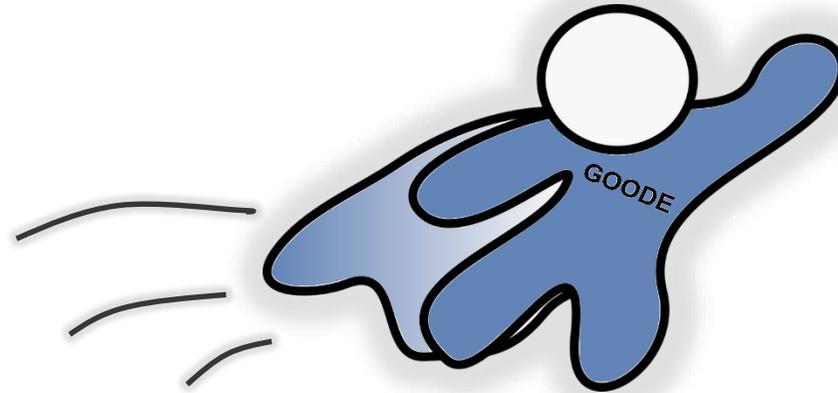
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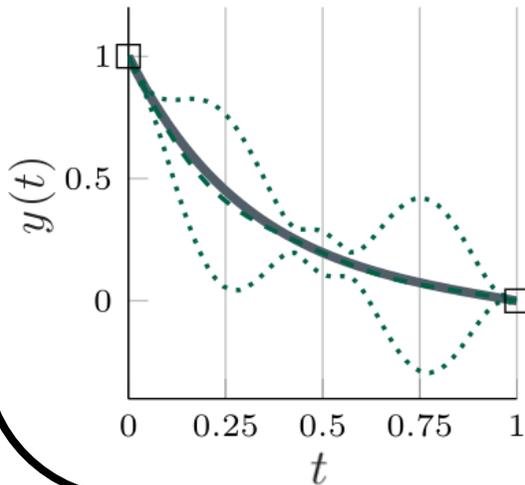
How does GOODE work?

Gaussian Process regression for linear BVP

[Owhadi 2015; 2017], [Cockayne 2016]

$$\left[\frac{d}{dt} - A\right]y(t) = q(t)$$

$$P(y(t)) = GP(m(t), k(t, t') \otimes V)$$



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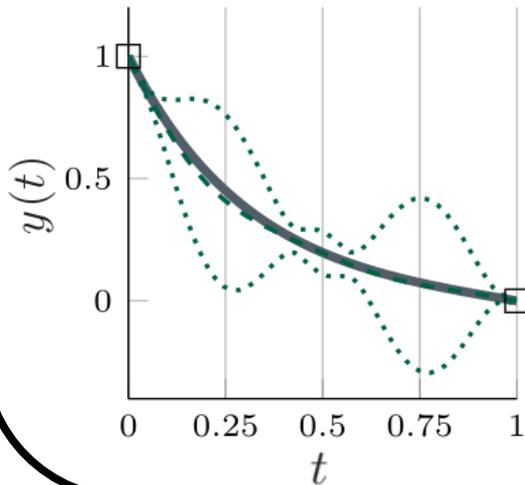
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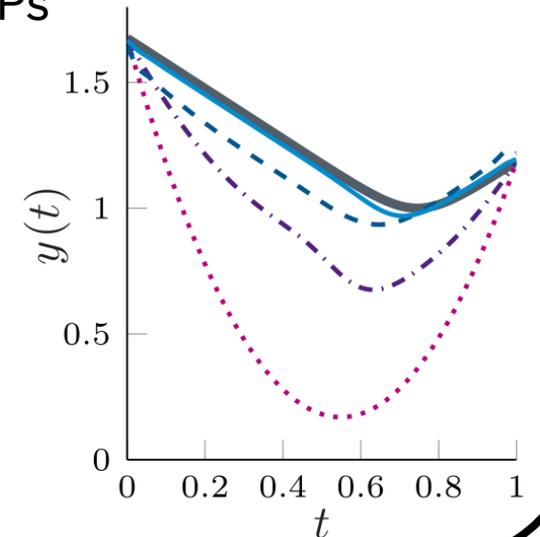


Quasilinearization of nonlinear BVP

[Bellman, Kalaba 1965]

Newton's method in function space

► Series of linear BVPs



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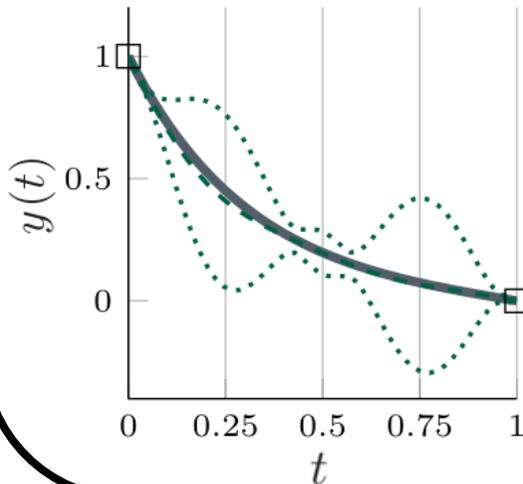
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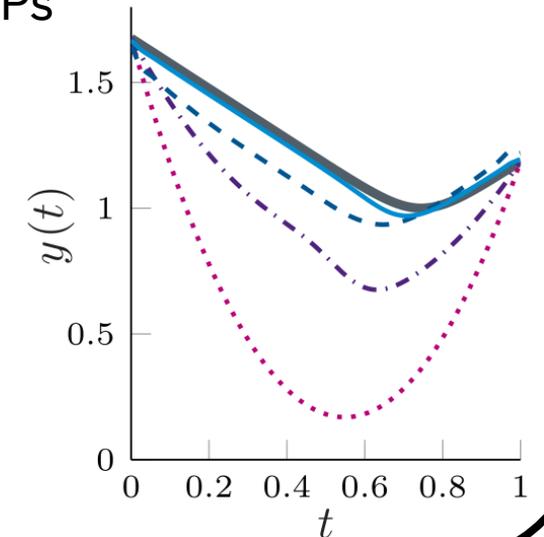


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GOODE

Iteratively approximate nonlinear problem

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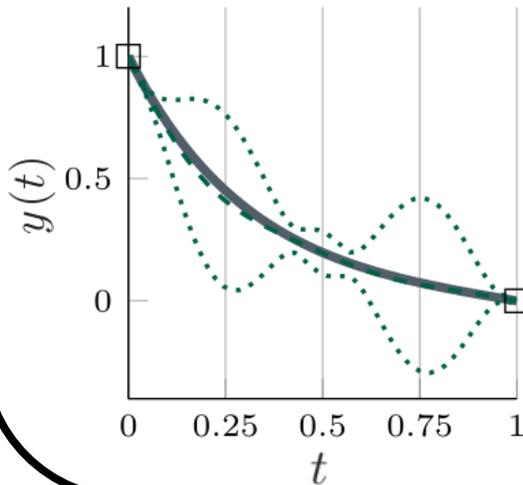
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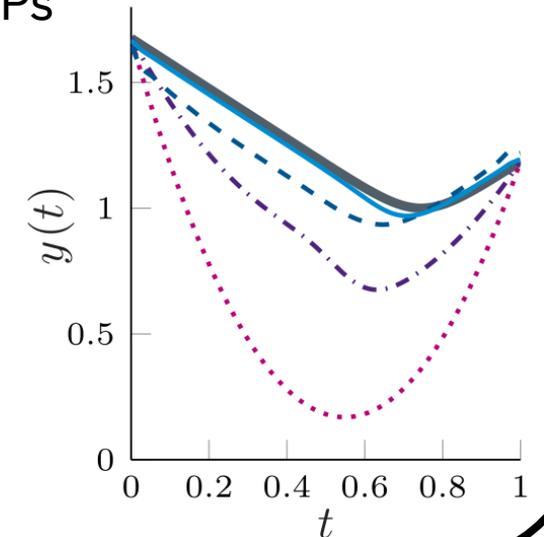


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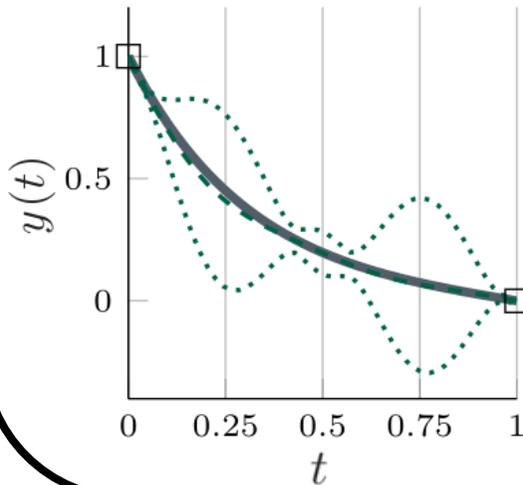
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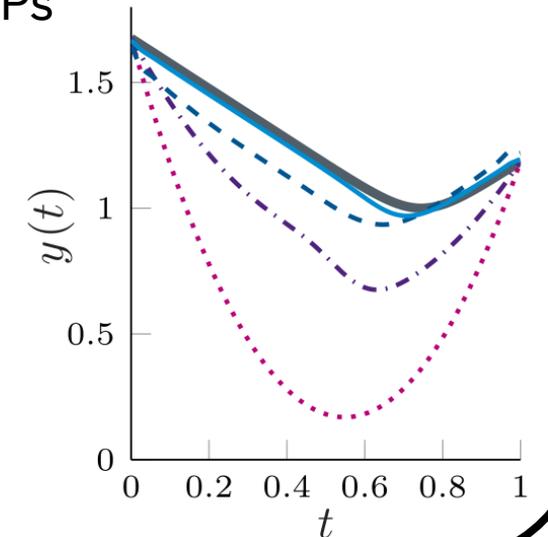


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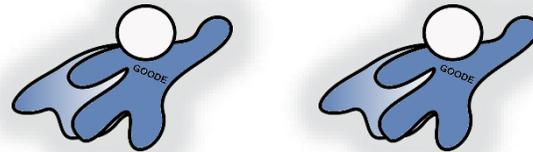
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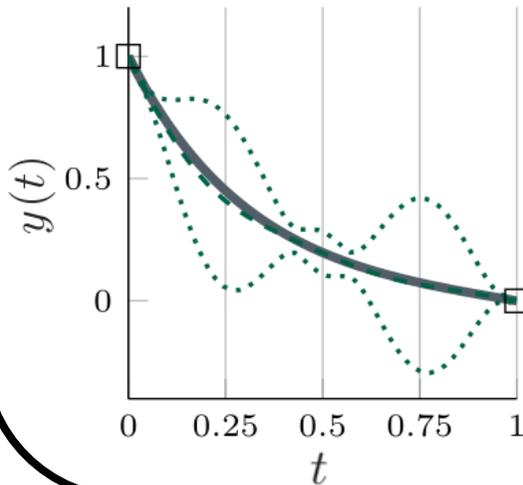
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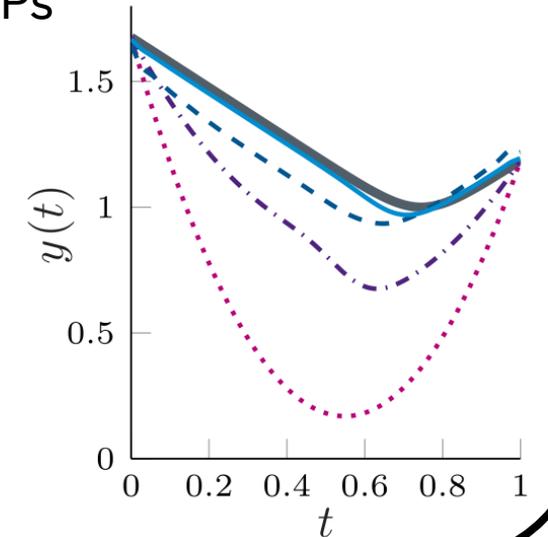


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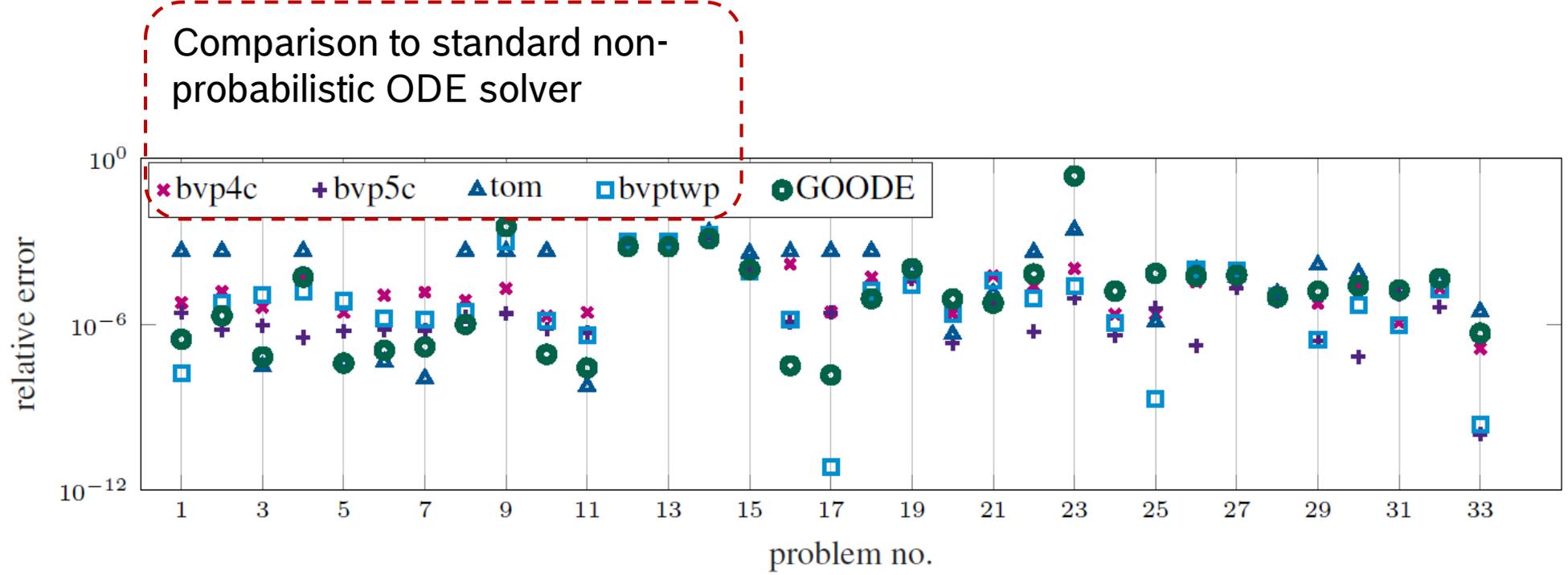
Iteratively approximate nonlinear problem



Return predictive posterior GP

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How good does GOODE work?



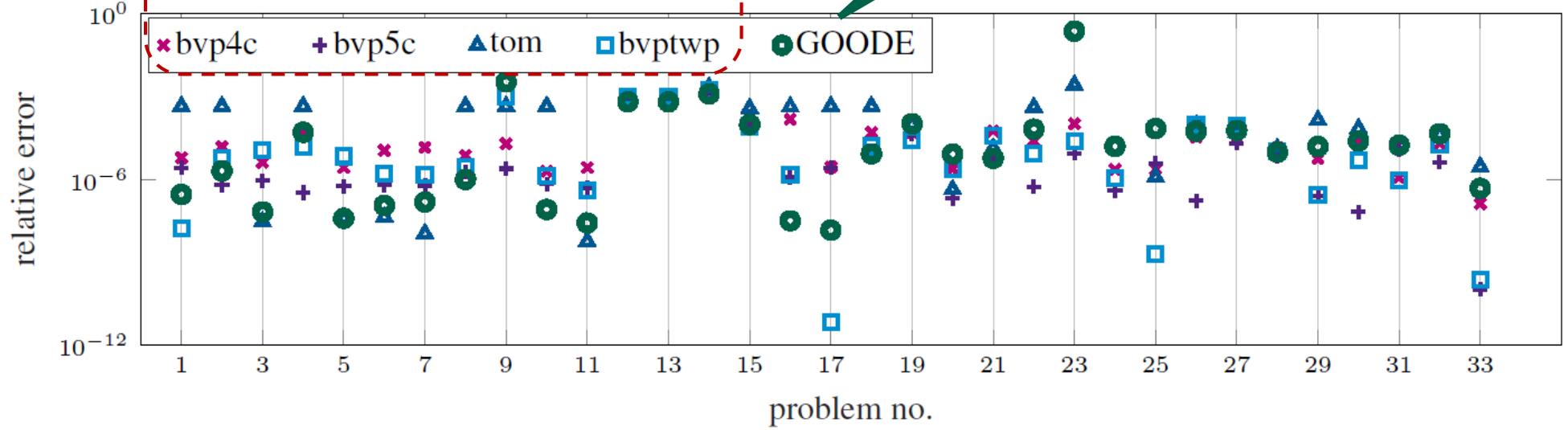
Testset of 33 problems [Mazzia 2014]

GOODE: A Gaussian Off-The-Shelf ODE Solver

How good does GOODE work?

Comparison to standard non-probabilistic ODE solver

Comparable in accuracy!
But with additional cost of kernel hyper-parameter optimization



Testset of 33 problems [Mazzia 2014]

GOODE: A Gaussian Off-The-Shelf ODE Solver

Want to know more?

Matlab code @ github.com/boschresearch/GOODE

The poster is divided into several sections:

- Introduction**: Discusses Ordinary differential equations (ODEs), Probabilistic Numerical Methods (PNM), and Boundary Value Problems (BVP).
- Gaussian Processes (GPs)**: Explains multi-output GP regression, prior GP distributions, and predictive posterior GP.
- Solving Linear BVPs with GPs**: Details the joint prior distribution, predictive posterior GP, and predictive posterior mean, covariance, and standard deviation.
- GOODE: A Gaussian Off-The-Shelf Ordinary Differential Equation Solver**: The main title of the poster.
- Authors**: David N. John, Vincent Heuveline, Michael Schober.
- A GOODE for you?**: Provides the GitHub link and a call to check out the paper and Matlab code.
- Experiments**: Shows model selection results and a plot of the solution for a specific ODE.
- GOODE**: Describes the solver for linear BVPs, including its multi-step approximation, error analysis, and numerical stability.
- Solving Nonlinear BVPs by Quasi-linearization**: Discusses the linearization of the BVP and the resulting series of linear BVPs.
- References**: Lists academic papers related to the work.



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- Introduction:** Discusses Ordinary differential equations (ODEs) and Probabilistic Numerical Methods (PNM).
- Boundary Value Problem (BVP):** Explains two-point BVPs and the shooting method.
- Gaussian Processes (GPs):** Details multi-output GP regression and predictive posterior GP.
- Solving Linear BVPs with GPs:** Shows the joint prior distribution and predictive posterior GP.
- Solving Nonlinear BVPs by Quasi-linearization:** Describes the linearization of the BVP.
- GOODE:** A Gaussian Off-The-Shelf Ordinary Differential Equation Solver. Includes a 3D surface plot and error analysis.
- Experiments:** Shows a plot of error vs. number of samples.
- References:** Lists academic papers related to the work.

THANK YOU!

