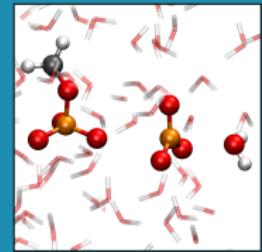


Ab Initio Molecular Dynamics Simulations of Phosphate Hydrolysis Using Neural Network Potentials



Master's thesis defence presentation

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Supervisor: Prof. J. Harvey

June 2025

1 Outline

- ① Introduction
- ② Theoretical background
- ③ Methodology
- ④ Results
- ⑤ Itemization and enumeration
- ⑥ Blocks and other environments

1 Why is phosphate hydrolysis challenging to study?

Complex Reaction Mechanism

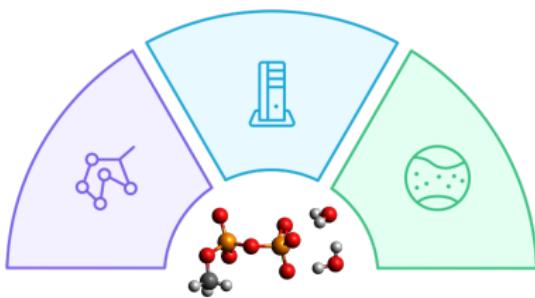
Involves multiple pathways and difficult-to-characterise transition states.

High Computational Cost

AIMD is expensive since it requires extensive sampling and large system sizes due to water's role.

Strong Solvent Effects

Complicated by hydrogen bonding and proton transfer in aqueous environments.



Would be nice to include a take-home message.

1 Research goals

- ▶ Compose a comprehensive dataset covering all reaction steps.
- ▶ Train the NequIP neural network to fit a neural network potential (NNP).
- ▶ Assess the accuracy and performance of the NNP.
- ▶ Perform well-tempered metadynamics simulations to obtain the free energy surface.
- ▶ Gain insights into the kinetics and thermodynamics of the reaction.
- ▶ Gain insights into the proton transfer mechanism.



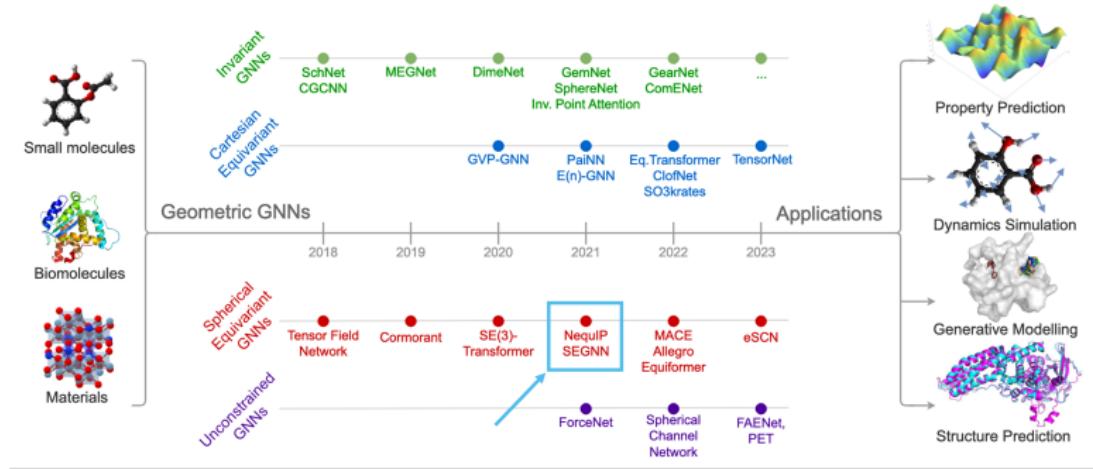
*It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems **without too much computation**.*

– Paul Dirac

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2 Geometric graph neural networks



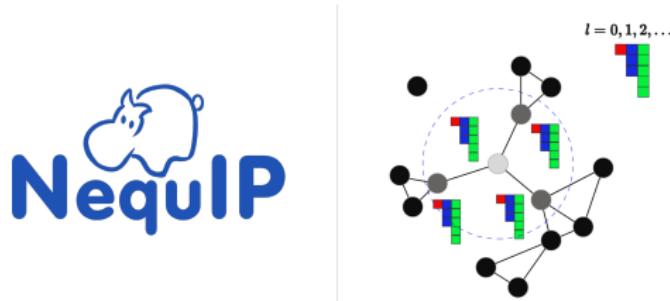
Would be nice to include a take-home message.

2 Neural equivariant interatomic potentials (NequIP)

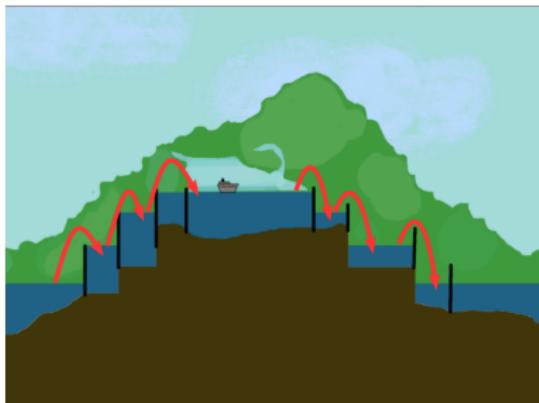
The neural network is trained using a loss function:

$$\mathcal{L} = \lambda_E \|\hat{E} - E\|^2 + \lambda_F \frac{1}{3N} \sum_{i=1}^N \sum_{\alpha=1}^3 \left\| -\frac{\partial \hat{E}}{\partial r_{i,\alpha}} - F_{i,\alpha} \right\|^2$$

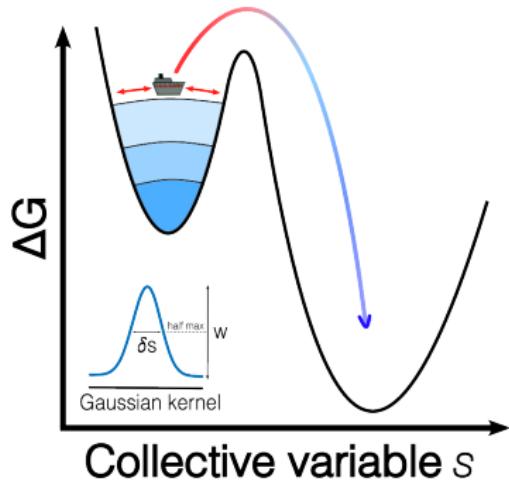
It is based on a weighted sum of energy and force loss terms. Where \hat{E} is the predicted energy, λ_E and λ_F are the energy and force weights, respectively, and N is the number of atoms. MSE loss is used.



2 Metadynamics



The Panama Canal

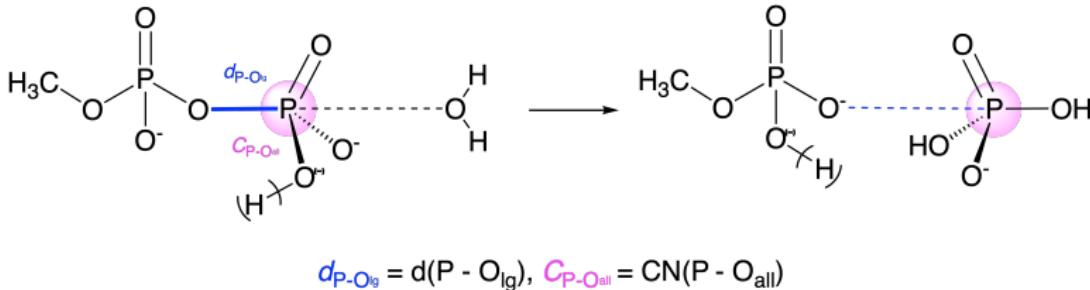


Would be nice to include a take-home message.

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3 System

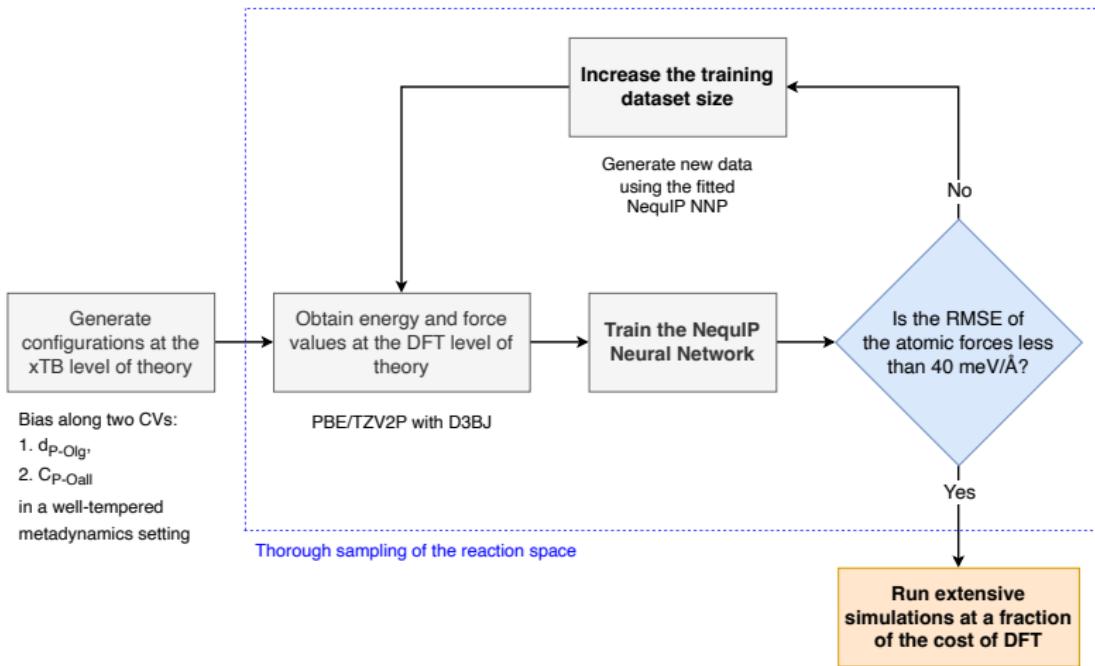


The systems studied in this work are the following:

- ▶ MeDP³⁻ with 3 Na⁺ counterions solvated by 119 H₂O.
- ▶ MeHDP²⁻ with 2 Na⁺ counterions solvated by 124 H₂O.

The box dimensions are 15.877 × 15.877 × 15.877 and 15.901 × 15.901 × 15.901 Å³, respectively.

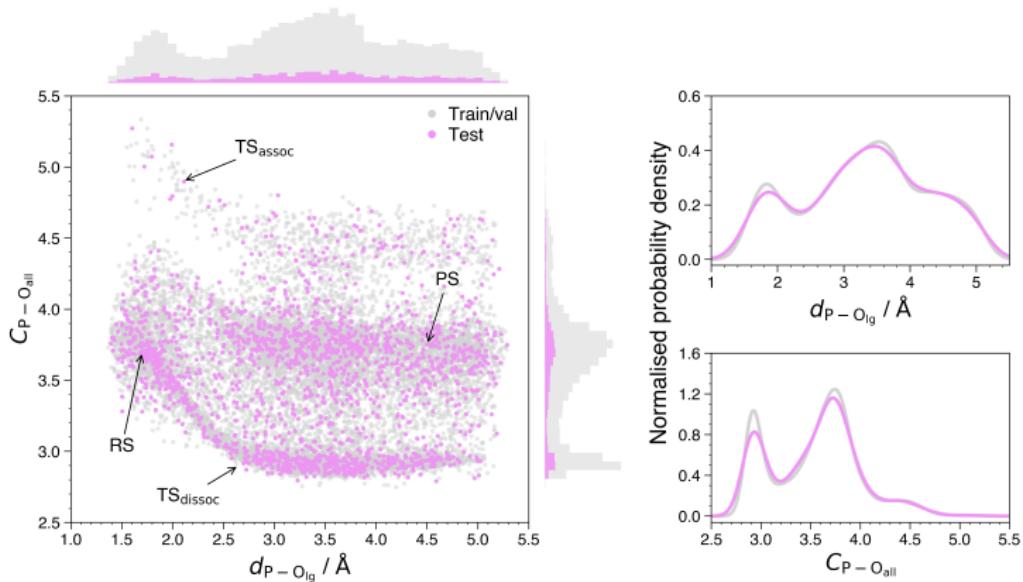
3 Neural network training workflow



4 Outline

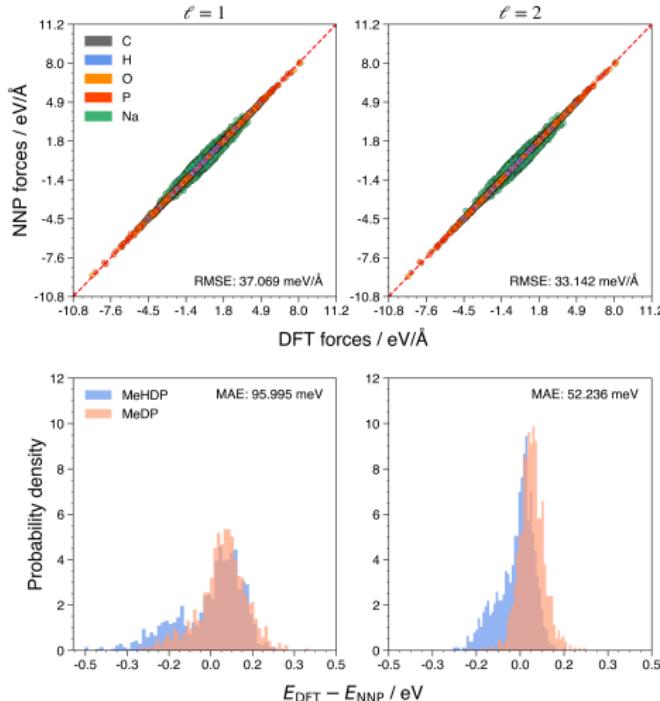
- ① Introduction
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4 Final training and test datasets' composition



The final training and test datasets consist of 12,000 and 1,800 frames, respectively, and covers all reaction steps.

4 Accuracy of the fitted potential

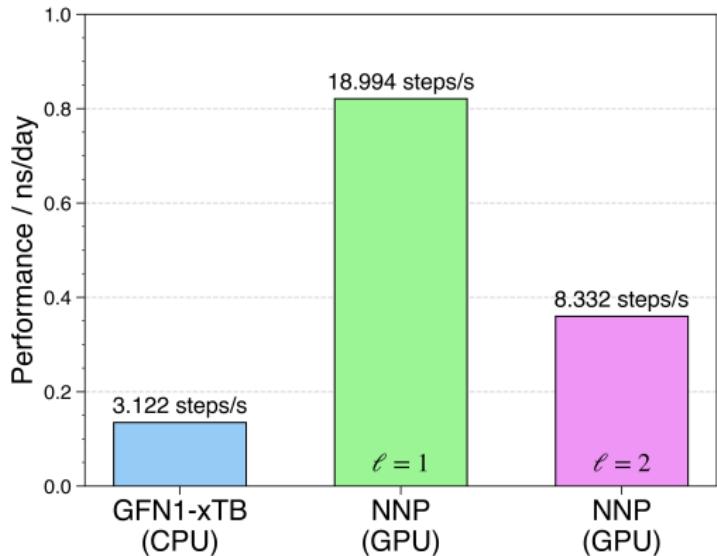


Community standards are as follows:

- ▶ ‘very good fit’
 $\text{MAE}_E = 1\text{-}10 \text{ meV/atom}$
 $\text{RMSE}_F = 20\text{-}40 \text{ meV/}\text{\AA}$
- ▶ ‘perfect fit’
 $\text{MAE}_E \sim 1 \text{ meV/atom}$
 $\text{RMSE}_F \sim 10 \text{ meV/}\text{\AA}$

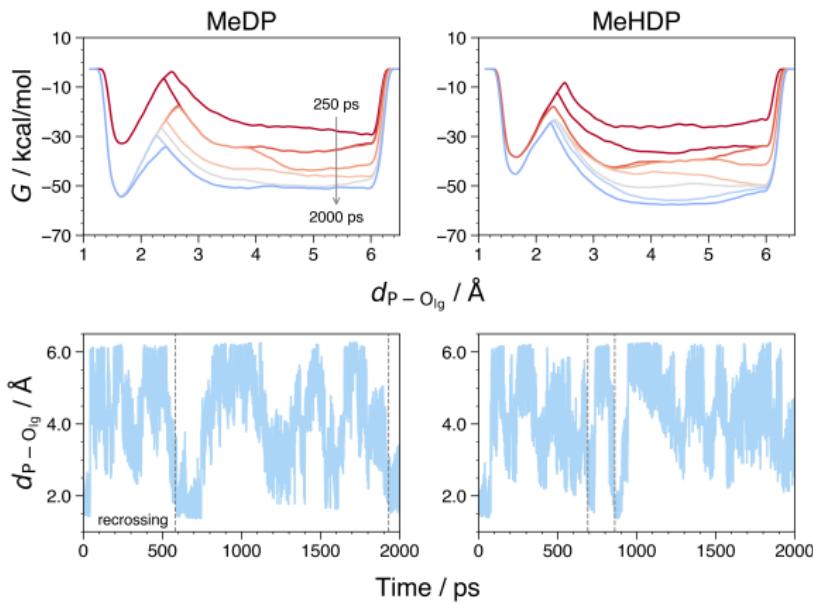
We fitted 2 potentials and both of them are very accurate exhibiting fairly small errors.

4 Performance of the potential



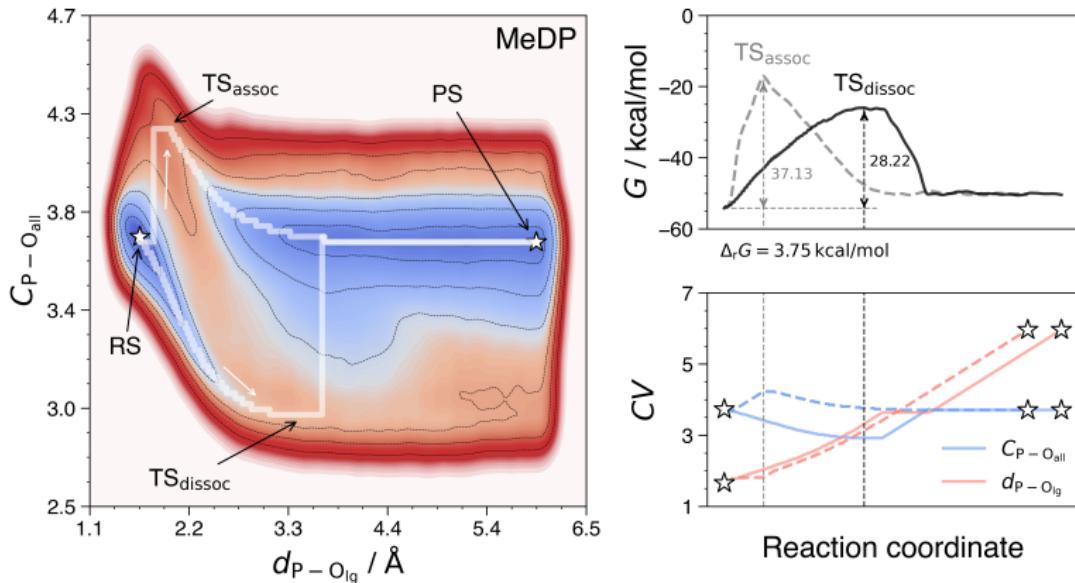
The turning point in choosing between the potentials with tensor ranks $\ell = 1$ and $\ell = 2$ is the performance. The $\ell = 1$ potential is about 2.5 times faster than the $\ell = 2$ potential, while the accuracy is comparable.

4 Convergence of the free energy profiles

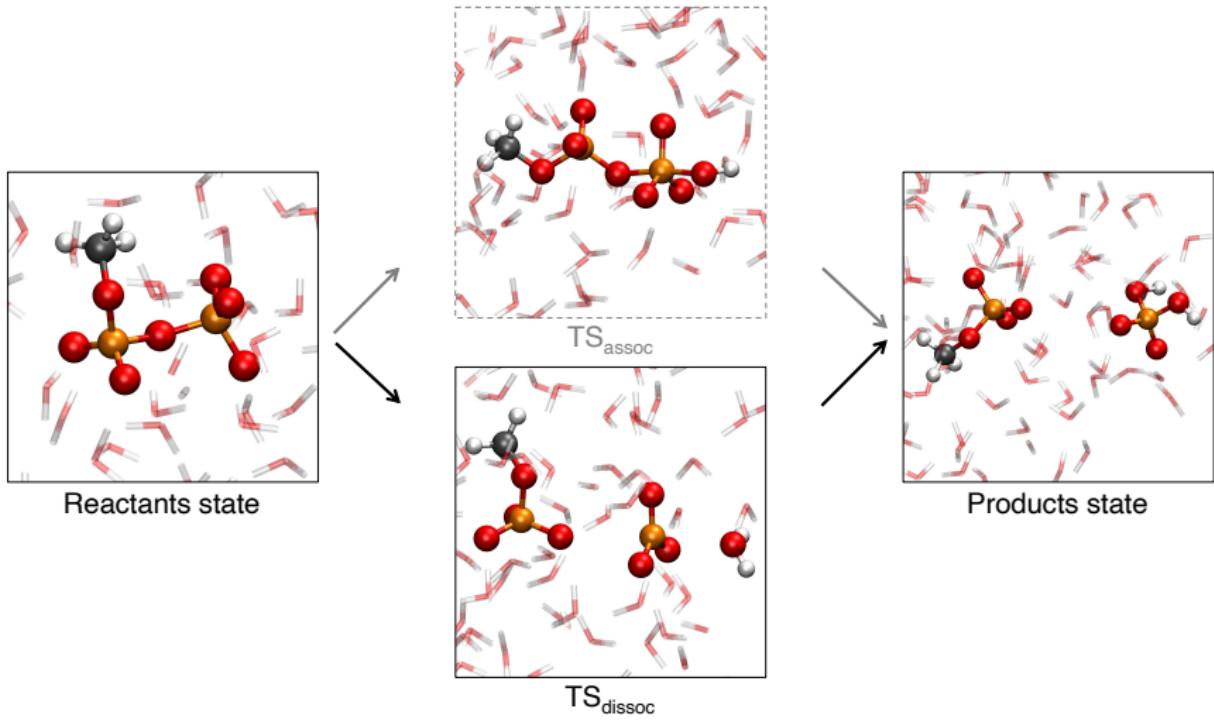


- ▶ The profiles are not fully converged.
- ▶ Hence, the results should be considered provisional.
- ▶ There are recrossing events between the reactants and products states.
- ▶ Which gives confidence in the soon approaching convergence.

4 Reaction mechanism for MeDP³⁻ at 300 K



The more favourable reaction mechanism is a dissociative/concerted ($D_N A_N$) one. $\Delta G_{\text{exp}}^{\ddagger}$ for $\text{HP}_2\text{O}_7^{3-}$ hydrolysis at 25°C is 29.2 kcal/mol. The $\Delta G_{\text{calc}}^{\ddagger}$ of 28.22 kcal/mol is within the chemical accuracy!



4 Positioning

Frame option [b] for text at the bottom of the frame

4 Footline

Frame option [plain] to remove footline on individual frame

To remove footline from *all* frames delete this line from preamble in .tex file:

```
\setbeamertemplate{footline}{body}
```

This frame has no title.

4 Double-column frame

This is the top of the first column.

This is the top of the second column.

4 Text alignment

Left justified environment ...

Center environment ...

Right justified environment ...

Ragged right command ...

Centering command ...

Ragged left command ...

Flush left command ...

Flush right command ...

4 Colour palette

Recommended, predefined colours

- ▶ black
- ▶ KU Leuven primary blue, secondary blue, and dark blue
- ▶ ← white, when background is dark
- ▶ 50% gray , for text and 5% gray for background
- ▶ red text colour, used for alert text

4 Font styles

Sans-serif family of Modern Latin font

- ▶ Normal text
- ▶ **Bold**
- ▶ *Italic, Emphasis, Slanted*
- ▶ Underline
- ▶ SMALL CAPS
- ▶ Typewriter

4 Font sizes

- ▶ tiny
- ▶ scriptsize
- ▶ footnotesize
- ▶ small
- ▶ normalsize
- ▶ large
- ▶ Large
- ▶ LARGE
- ▶ huge
- ▶ Huge

4 Equations and math

Equations and other mathematical symbols use serif typeface:

$$f(x) = ax^2 + bx + c$$

Style of individual symbols can be changed manually:

$$\hat{\beta} = \arg \min_b (\mathbf{y} - \mathbf{X}\mathbf{b})^\top \boldsymbol{\Omega}^{-1} (\mathbf{y} - \mathbf{X}\mathbf{b})$$
$$G_t = \alpha e^{-\beta e^{-\gamma \cdot t}}$$

To change all math into sans-serif delete this line from the preamble in .tex file:

```
\usefonttheme[onlymath]{serif}
```

4 Graphics

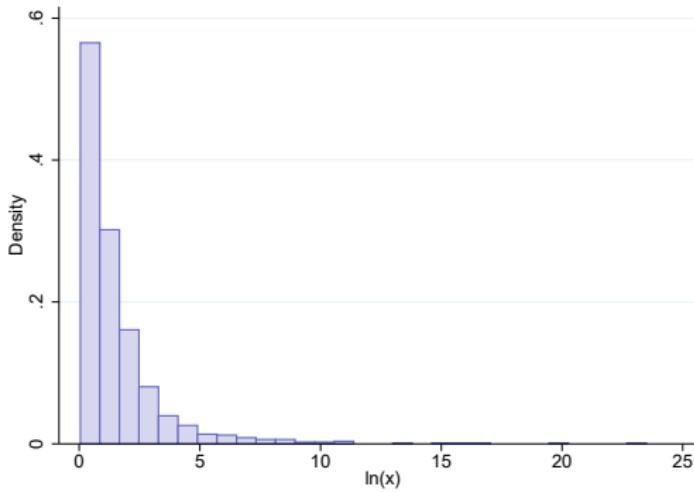


Figure: Example graphic

Do not delete logo files in the graphics folder. They are used on the title page and in the footnote.

4 Tables

Table: Example table

	(1)	(2)	(3)
x_1	0.705*** (0.107)	0.215** (0.0964)	0.123 (0.105)
x_2	0.476*** (0.0489)		0.114** (0.0519)
x_3		0.592*** (0.0361)	0.538*** (0.0436)
Constant	0.0478 (0.0487)	0.0576 (0.0427)	0.0511 (0.0426)
Observations	500	500	500
R-squared	0.711	0.776	0.779

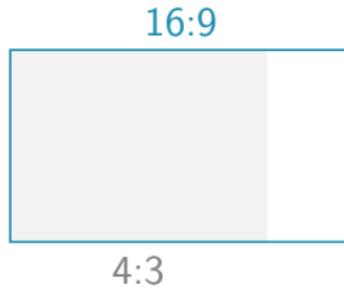
Standard errors in parentheses, *** p<0.01, ** p<0.05, * p<0.1

4 Widescreen

Default screen ratio is 4:3. Load the following package in the preamble to make all frames wider to 16:9 ratio:

```
\usepackage[orientation=landscape,size=custom,  
width=16,height=9,scale=0.5,debug]{beamerposter}
```

Title page or other frames should not get distorted because of it.



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5 Itemize

(default)

- ▶ Itemize style
- ▶ Itemize style
 - Itemize subitem
 - Itemize subitem
 - Itemize subsubitem
 - Itemize subsubitem
 - Itemize subitem
- ▶ Itemize style

5 Itemize

(extra space between items)

- ▶ Itemize style
- ▶ Itemize style
 - Itemize subitem
 - Itemize subitem
 - Itemize subitem
- ▶ Itemize style

5 Enumerate

(default)

- 1 Enumerate style
- 2 Enumerate style
 - 1 Enumerate subitem
 - 2 Enumerate subitem
 - 1 Enumerate subsubitem
 - 2 Enumerate subsubitem
 - 3 Enumerate subitem
- 3 Enumerate style

5 Enumerate

(option I) + pause

- I Enumerate style
- II Enumerate style
 - I Enumerate subitem
 - II Enumerate subitem

5 Enumerate

(option I) + pause

- I Enumerate style
- II Enumerate style
 - I Enumerate subitem
 - II Enumerate subitem
 - I Enumerate subsubitem
 - II Enumerate subsubitem

5 Enumerate

(option I) + pause

- I Enumerate style
- II Enumerate style
 - I Enumerate subitem
 - II Enumerate subitem
 - I Enumerate subsubitem
 - II Enumerate subsubitem
 - III Enumerate subitem
- III Enumerate style

5 Enumerate

(option i.)

- i. Enumerate style
- ii. Enumerate style
 - i. Enumerate subitem
 - ii. Enumerate subitem
 - i. Enumerate subsubitem
 - ii. Enumerate subsubitem
 - iii. Enumerate subitem
- iii. Enumerate style

5 Enumerate

(option A.) + effects

- A. Enumerate style
- B. Enumerate style

5 Enumerate

(option A.) + effects

- A. Enumerate style
- B. Enumerate style
 - A. Enumerate subitem

5 Enumerate

(option A.) + effects

- A. Enumerate style
- B. Enumerate style
 - A. Enumerate subitem
 - B. Enumerate subitem
 - A. Enumerate subsubitem
 - B. Enumerate subsubitem

5 Enumerate

(option A.) + effects

- A. Enumerate style
- B. Enumerate style
 - A. Enumerate subitem
 - B. Enumerate subitem
 - A. Enumerate subsubitem
 - B. Enumerate subsubitem
- C. Enumerate subitem

5 Enumerate

(option A.) + effects

- A. Enumerate style
- B. Enumerate style
 - A. Enumerate subitem
 - B. Enumerate subitem
- C. Enumerate subitem
- C. Enumerate style

5 Enumerate

(option a + extra space)

- a Enumerate style
- b Enumerate style
 - a Enumerate subitem
 - b Enumerate subitem
 - a Enumerate subsubitem
 - b Enumerate subsubitem
 - c Enumerate subitem
- c Enumerate style

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6 Theorems and other blocks

Title of the bloc

Text for generic block

Example block title

Text for example block

Alert block title

Text for alert block

6 Theorems and other blocks

Theorem environment

Theorem

$$a^2 + b^2 = c^2$$

Definition environment

Definition

Here is definition text

Example environment

Example

Example text

6 Theorems and other blocks

Proof environment

Proof.

Proof text.



Proof with custom title

Proof with any name and optionally without full stop in the title



Corollary environment

Corollary

$$x + y = y + x$$

6 Boxes

'Beamer color box' with five different pre-set colour combinations

box1 scheme

box2 scheme

second line

box3 scheme,
aligned right

box4 scheme,
aligned left

box5

6 Quotes

Quote

Quote environment is for a short quotation, or a series of small quotes, separated by blank lines.

Quotation

Quotation environment is for use with longer quotations, of more than one paragraph, because it indents the first line of each paragraph.

Quotation environment is for use with longer quotations, of more than one paragraph, because it indents the first line of each paragraph.

– WikiBooks \LaTeX guide

6 Quotes

Verse

*Verse environment
is for quotations where
line breaks are important.*

Verbatim

Verbatim text is ideal for typesetting program source code. To use it in Beamer the frame needs option [fragile].

Abstract environment

Abstract

Lore*m ipsum dolor sit amet, consectetur adipiscing elit.*

Pellentesque quis pharetra sapien, non tempor tortor. Vestibulum gravida mauris ac lorem semper, vel vulputate mauris tincidunt. Sed diam ante, dignissim consequat pulvinar in, placerat eu nibh. Donec congue id elit sit amet iaculis.

Proin pellentesque vel ex in fermentum. Pellentesque suscipit odio ut accumsan feugiat. Aliquam erat volutpat. Sed feugiat cursus eros, sit amet vestibulum ipsum pulvinar at. Sed eget porttitor purus. Duis nec nunc ex. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae.

6 Buttons

Standard buttons

[Link to Figure 1](#)

[▶ Extra frame](#)

[▶▶ Button with long title and no link](#)



These buttons can link to any frame, figure, table, theorem, section, or anything else with defined label

Ending frame (version 1)

Ending frame (version 2)

6 Extra slide

Because of frame option [noframenumbering] this frame is not counted in the total number of frames.

This button with cross-referencing link that will take you back to the frame:

[◀ Back to Buttons](#)