Applied AI Tools for Scientific Programming

Scientific workflows: Tools and Tips 🛠️

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What is this lecture series?

Scientific workflows: Tools and Tips 🛠️

🗓️ Every 3rd Thursday 🕓 4-5 p.m. 📍 Webex

- One topic from the world of scientific workflows
- Material provided online
- If you don't want to miss a lecture subscribe to the mailing list
- For credit points: Send me a short message (Email or Webex)

Motivation

- Speed up repetitive tasks
- Learn new methods and languages
- Support debugging, documenting, refactoring, ...

AI tools for programming

- Browser-based chat bots (ChatGPT, etc.)
- Web-tools for data analysis (Data analyst GPT, JuliusAI, …)
- **IDE-integrated AI tools** (GitHub Copilot, Codium AI, …)

Integrated tools

- know your project structure
- see your code and console output
- respond in context while coding

Today

GitHub Copilot inside the IDE Positron

- How to use it
- Limitations and responsible use

Let’s get started

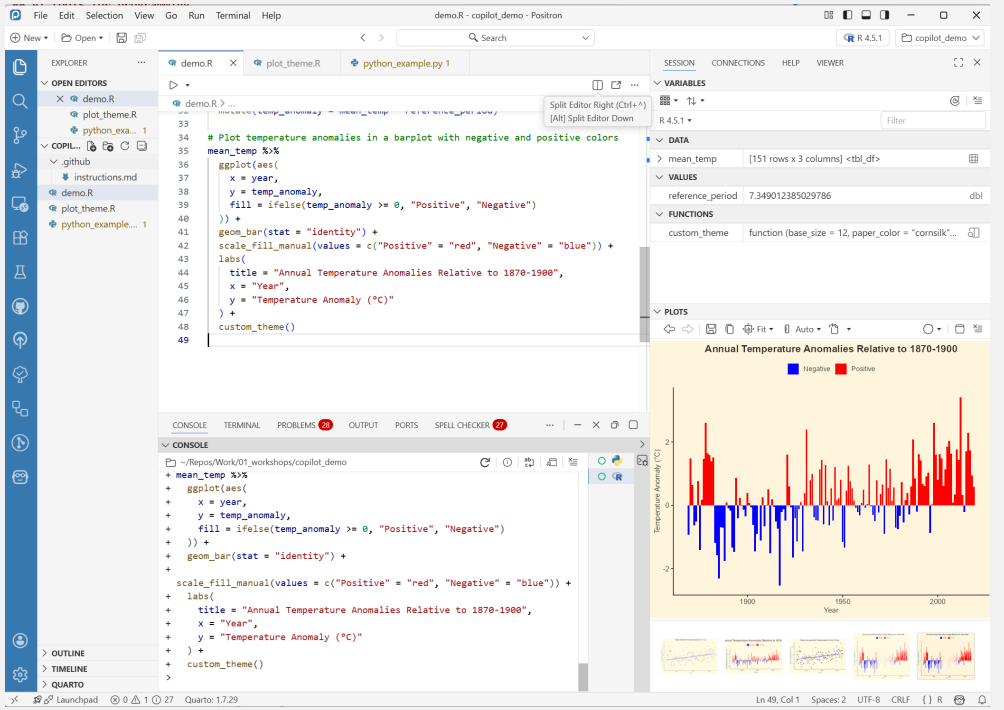
GitHub Copilot in Positron

GitHub Copilot

- **Integrated** and **context-aware**
- **Standard** tool for different environments
- **Free** for academics with an educational account
  - See lecture website for guide on how to get it

Positron

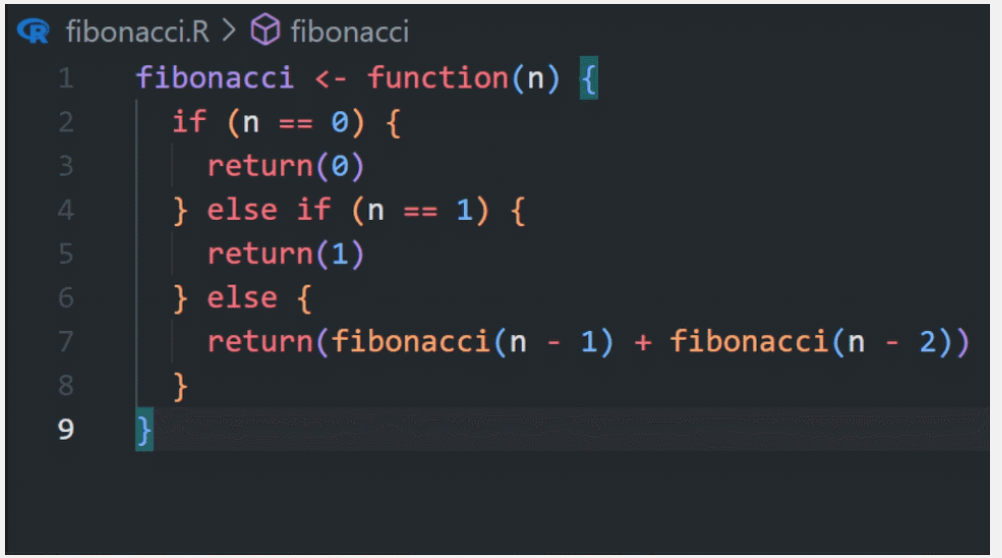
- General-purpose data science IDE
- Built by the same team behind RStudio
- Based on VS Code
- Complete GitHub Copilot integration



Code auto-complete

Copilot predicts what you want to write based on

- Current code
- Open files
- Comments

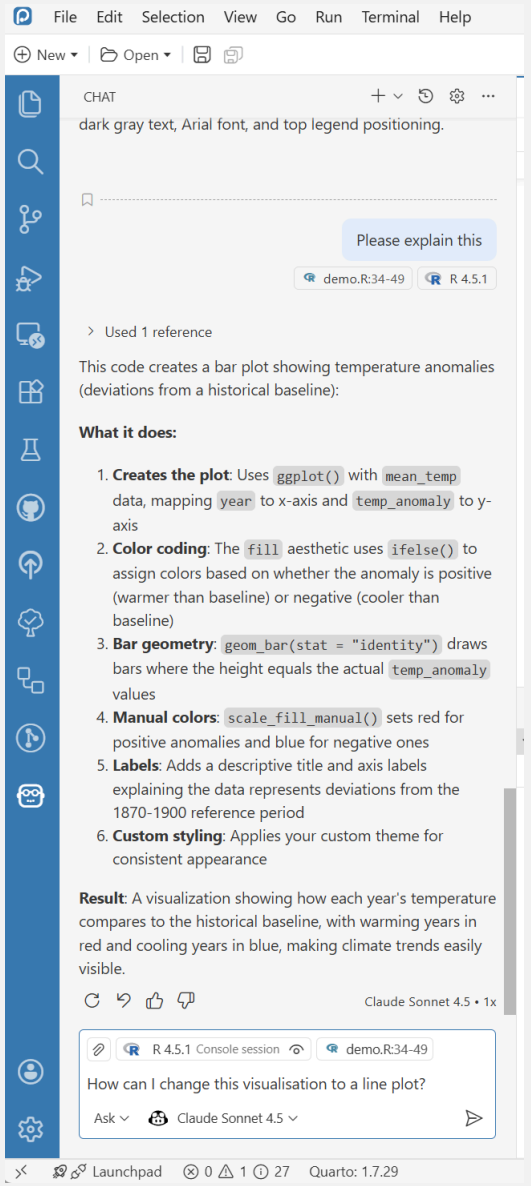


Get better suggestions

- Provide context
  - Good comments and names for functions and variables
  - Open other relevant files
- Adopt a good coding style
  - GitHub Copilot will imitate your style
- Acceptance discipline
  - Don’t auto-accept everything
  - Modify suggestions if needed

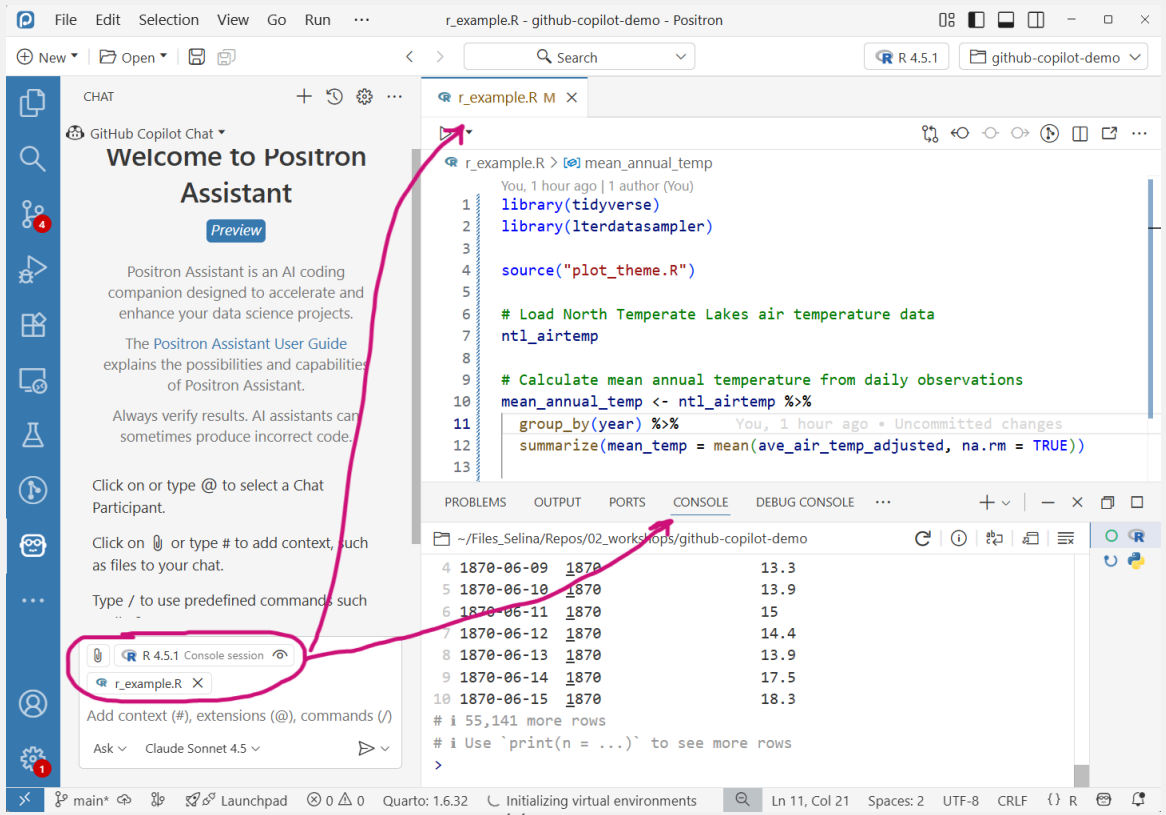
Sidebar Chat

- Tell GitHub Copilot what to do with your code
- Larger contexts and longer conversations
- Can see: files, console output, project workspace



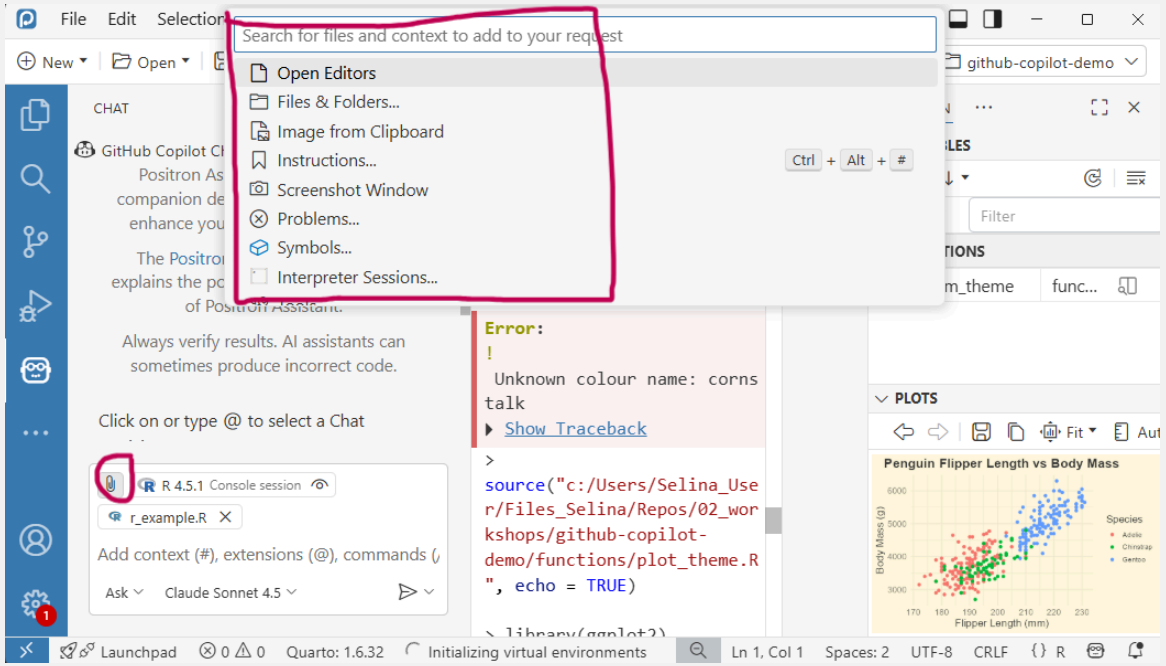
The default context

- Context is indicated at the top of the chat
- Default context: current file + console output
- If you highlight code, the highlighted code is added as context



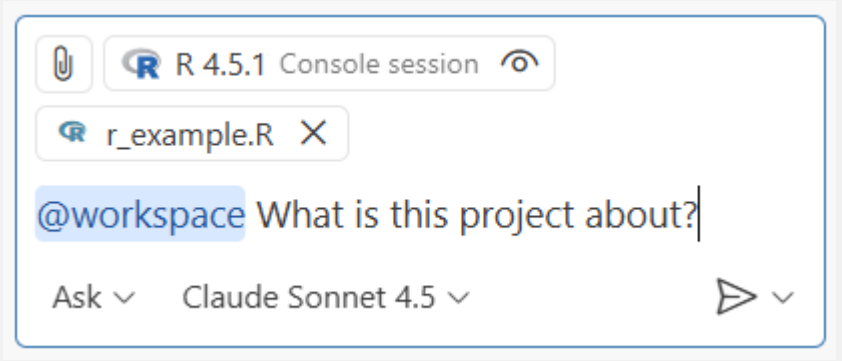
The “Add context” button

- Add other files and folders as context with the “Add context” button

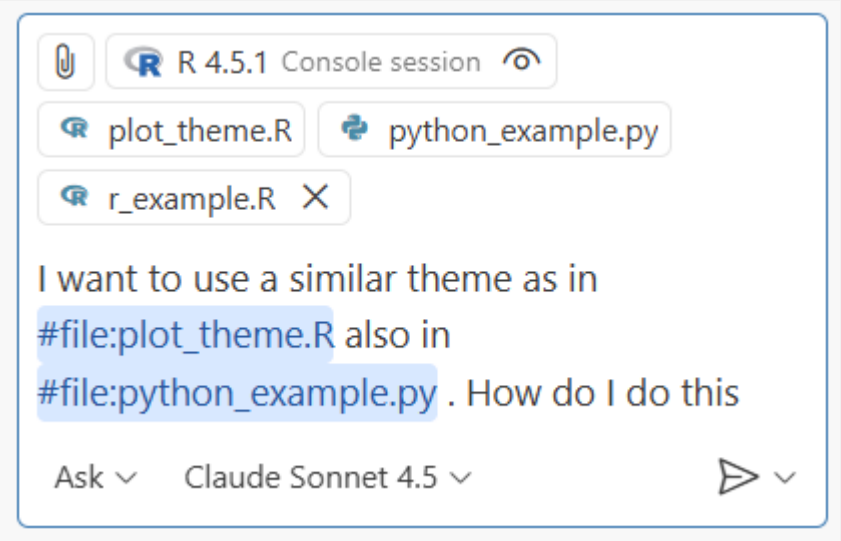


Use @, # or copy-paste

`@workspace` adds all files in the project



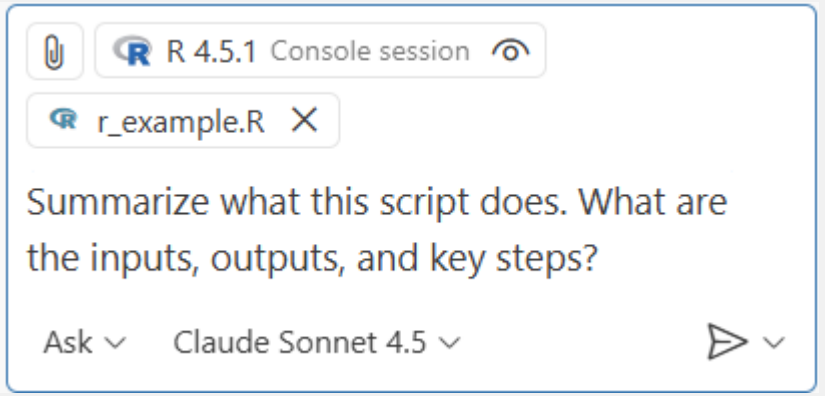
`#file` adds specific files to the context



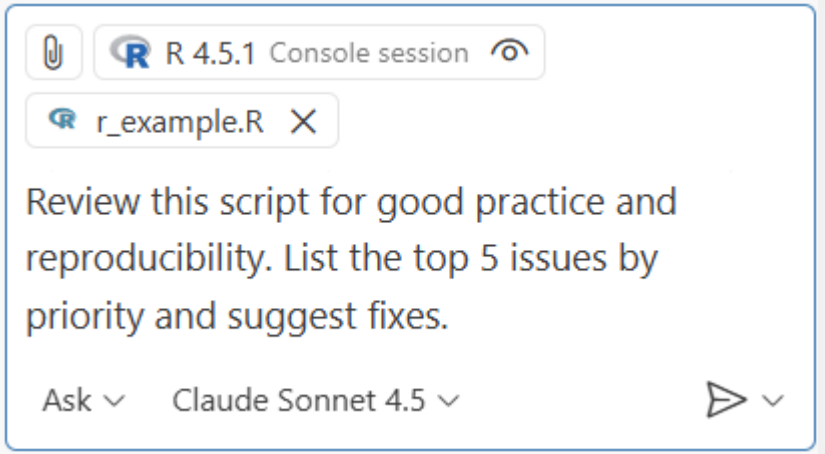
You can also copy paste images (e.g. screenshots) as context in the chatbox

Sidebar chat: prompt ideas

Overview of unfamiliar scripts

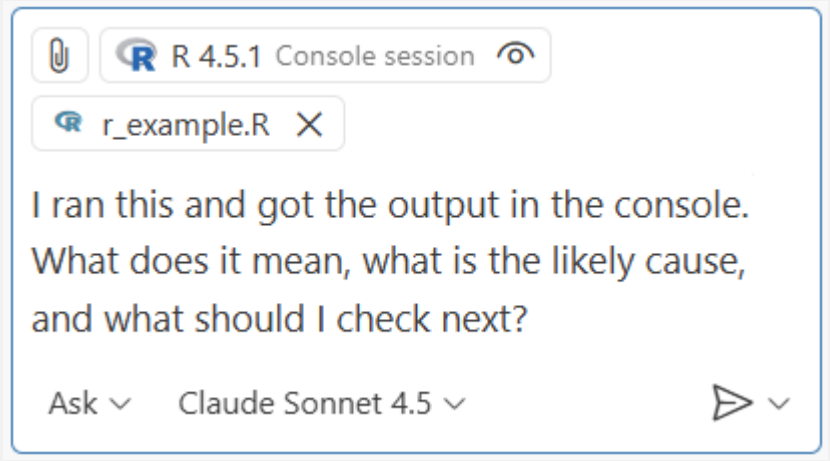


Review your own code

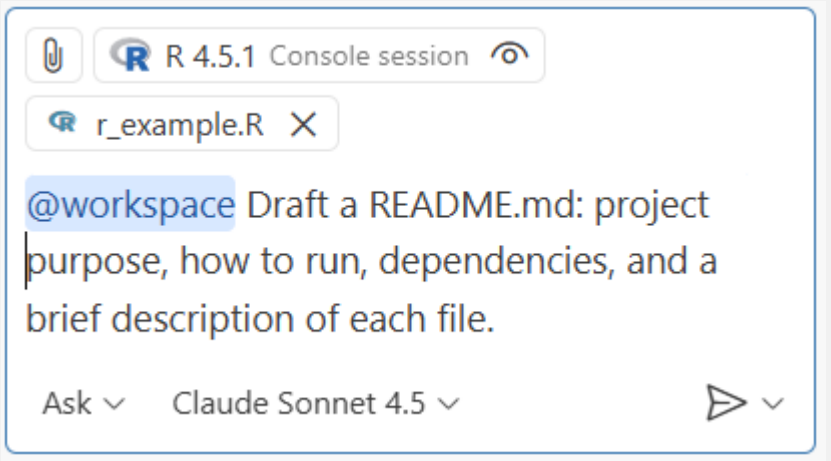


Sidebar chat: prompt ideas

Understand output (errors, warnings, surprising results)



Write project-level documentation draft



Advanced features

- Project-level instruction files
  - Give instructions that apply to the whole project
  - Special file in `/.github/instructions.md`
- Agents: Automate multi-step workflows (use with care)

Limitations and risks

- Can suggest
  - Outdated functions and code
  - Patterns that are common but not best practice
- GitHub Copilot has no understanding
- Predicts plausible code not necessarily correct code
  - Code can be subtly wrong or inappropriate
- Risk of over-reliance

Responsible use

- Don’t treat AI as an authority: review and double-check
- Use version control as a safety net: review and trace changes
- Privacy: Code, comments and console output may be shared with model providers
  - Beware if you have sensitive data
- Check institutional and journal guidelines
- Transparency: Disclose your use of AI tools
- You are responsible for your scientific output

Conclusion

- GitHub Copilot can be a great **assistant**
- Support but not replace

Getting started

1. Get GitHub Copilot for free with your educational GitHub account
2. Install Positron
3. Setup GitHub Copilot in Positron

Check out the lecture website for all relevant information

Next lecture

Topic t.b.a.

🗓️ 15th January 🕓 4-5 p.m. 📍 Webex

🔔 Subscribe to the mailing list

📧 For topic suggestions and/or feedback send me an email

Thanks for your attention :)

Questions?