hw01

April 9, 2025

[1]:
```
from typing import Union, Optional
from enum import Enum

import numpy as np
import matplotlib.pyplot as plt
from scipy.optimize import minimize
import pdb

np.set_printoptions(linewidth=160)
np.random.seed(42)

POPULATION_PER_AGE = 1000
MAX_AGE = 50
NUM_YEARS = 50
GLOBAL_DEFAULT_A1 = 10
```

1 Catalytic Model:

1.1 Combination of work from class and extending the model for HW 1

[2]:
```
np.append(np.array([1, 0, 2]), 3)
```

[2]:
```
array([1, 0, 2, 3])
```

[3]:
```
class LambdaVariationMethod(Enum):
    """Enum for different methods of varying lambda."""
    YEAR = "year"
    AGE = "age"


def prepare_catalytic_model_config(
    lambda_variation_method: LambdaVariationMethod,
    lambda_variation_params: Union[np.ndarray, list[Union[float, int]]],
    include_births: bool = True,
    deterministic: bool = True,
) -> dict:
    """Prepare the configuration for the simulation."""
```

```
    if lambda_variation_method == LambdaVariationMethod.YEAR:
        config = {
            "lambda_variation_method": lambda_variation_method,
            "lambda_variation_params": {
                "lambda_by_year": lambda_variation_params
            },
            "include_births": include_births,
            "deterministic": deterministic,
        }
    elif lambda_variation_method == LambdaVariationMethod.AGE:
        if len(lambda_variation_params) < 2:
            raise ValueError("Not enough parameters provided for lambda␣
↪variation method.")
        elif len(lambda_variation_params) == 2:
            lambda_variation_params = np.append(lambda_variation_params,␣
↪GLOBAL_DEFAULT_A1)
        elif len(lambda_variation_params) > 3:
            raise ValueError("Too many parameters provided for lambda variation␣
↪method.")

        config = {
            "lambda_variation_method": lambda_variation_method,
            "lambda_variation_params": {
                "lambda_a": lambda_variation_params[0],
                "lambda_b": lambda_variation_params[1],
                "A_1": lambda_variation_params[2],
            },
            "include_births": include_births,
            "deterministic": deterministic,
        }
    else:
        raise ValueError("Invalid lambda variation method provided. No other␣
↪variation methods have benen implemented yet.")
    return config


# example_config_by_year = {
#     "lambda_variation_method": LambdaVariationMethod.YEAR,
#     "lambda_variation_params": {
#         "lambda_by_year": np.random.uniform(0.05, 0.15, NUM_YEARS)
#     },
#     "include_births": True,
#     "deterministic": True,
# }
# example_config_by_age = {
#     "lambda_variation_method": LambdaVariationMethod.AGE,
#     "lambda_variation_params": {
```

```
#         "lambda_by_age": {
#             "lambda_a": 0.3,
#             "lambda_b": 0.05,
#             "A_1": 10,
#         }
#     },
#     "include_births": True,
#     "deterministic": True,
# }
```

[4]:
```
def catalytic_model(
    config: Optional[dict],
    # lambda_by_year: Optional[np.ndarray] = None,
    # lambda_by_age_params: Optional[list[Union[int, float]]] = None,
    # include_births: bool = True,
    # deterministic: bool = True,
) -> np.ndarray:
    """
    :param lambda_by_year: Infection rate by year
    :param lambda_by_age_params: Infection rate by age
        This is a 1D array of length 3 where the entries are [lambda_a,␣
 ↪lambda_b, A_1]
        where lambda(a) = lambda_a if age <= A_1
        and lambda(a) = lambda_b if age > A_1
    :param include_births: Include births in the model
    :param deterministic: If True, use deterministic model

    :return: si_out: Susceptible and Infected by age group and year
    """
    # susceptible and Infected by age group and year
    si_out = np.zeros((NUM_YEARS+1, MAX_AGE+1, 3))

    # Initial first year
    si_out[0, :, 0] = POPULATION_PER_AGE

    if config["include_births"]:
        # 100 Births every year
        si_out[:, 0, 0] = POPULATION_PER_AGE

    if config["lambda_variation_method"] == LambdaVariationMethod.YEAR:
        lambda_by_year = config["lambda_variation_params"]["lambda_by_year"]
        lambda_by_year_and_age = np.repeat(lambda_by_year.reshape(-1, 1),␣
 ↪MAX_AGE, axis=1)

    elif config["lambda_variation_method"] == LambdaVariationMethod.AGE:
        lambda_variation_params = config["lambda_variation_params"]
```

```
        lambda_a = lambda_variation_params["lambda_a"]
        lambda_b = lambda_variation_params["lambda_b"]
        A_1 = (lambda_variation_params["A_1"] + 1).astype(int)

        # pdb.set_trace()

        lambda_by_age = np.zeros(MAX_AGE + 1)
        lambda_by_age[:A_1] = lambda_a
        lambda_by_age[A_1:] = lambda_b

        lambda_by_year_and_age = np.repeat(lambda_by_age.reshape(1, -1),␣
↪NUM_YEARS, axis=0)

    else:
        raise ValueError("Invalid lambda variation method provided. No other␣
↪variation methods have been implemented yet.")

    for y_num in range(NUM_YEARS):
        for a_num in range(MAX_AGE):
            curr_susceptible = si_out[y_num, a_num, 0]
            curr_infection = si_out[y_num, a_num, 1]

            curr_lamb = min(lambda_by_year_and_age[y_num, a_num], 1)

            if config["deterministic"]:
                created_infections = curr_susceptible * curr_lamb
            else:
                # TODO: In the future make this a binomial random variable␣
↪which uses
                #   this as a probability for each susceptible person to be␣
↪infected.
                raise NotImplementedError("Stochastic model not implemented yet.
↪")

            new_susceptible = curr_susceptible - created_infections
            new_infection = curr_infection + created_infections

            si_out[y_num + 1, a_num + 1, 0] = new_susceptible
            si_out[y_num + 1, a_num + 1, 1] = new_infection
            si_out[y_num, a_num, 2] = created_infections

    return si_out


def get_infections_by_year(
    si_out: np.ndarray,
) -> np.ndarray:
```

```
    """
    Get infections by year from the output of the catalytic model.

    :param si_out: Output of the catalytic model

    :return: Infections by year
    """
    return si_out[:NUM_YEARS, :MAX_AGE, 2].sum(axis=1)


def sum_squared_error(
    ground_truth: np.ndarray,
    best_guess: np.ndarray,
) -> float:
    return ((ground_truth - best_guess)**2).sum()


def objective_function(
    learned_params: np.ndarray,
    lambda_variation_method: LambdaVariationMethod,
    si_out_gt: np.ndarray,
    include_births: bool = True,
    deterministic: bool = True,
    population_wide_error: bool = True,
) -> float:
    """
    Objective function for optimization.

    :param learned_params: Parameters to be optimized various forces of␣
 ↪infection
    :param lambda_variation_method: Method of varying lambda either AGE or YEAR␣
 ↪for now
    :param infections_by_year_gt: Ground truth infections by year
    :param include_births: Include births in the model
    :param deterministic: If True, use deterministic model

    :return: Sum of squared errors between ground truth and guessed infections
    """
    config = prepare_catalytic_model_config(
        lambda_variation_method=lambda_variation_method,
        lambda_variation_params=learned_params,
        include_births=include_births,
        deterministic=deterministic,
    )
    si_out = catalytic_model(config)

    if population_wide_error:
```

```
        infections_guess = get_infections_by_year(si_out)
        infections_gt = get_infections_by_year(si_out_gt)

    else:
        infections_guess = si_out[:NUM_YEARS, :MAX_AGE, 2]
        infections_gt = si_out_gt[:NUM_YEARS, :MAX_AGE, 2]

    return sum_squared_error(infections_gt, infections_guess)
```

[5]:
```
lambda_by_year_gt = np.random.uniform(0.05, 0.15, NUM_YEARS)
config_gt = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.YEAR,
    lambda_variation_params=lambda_by_year_gt,
)
si_out_gt = catalytic_model(config_gt)
```

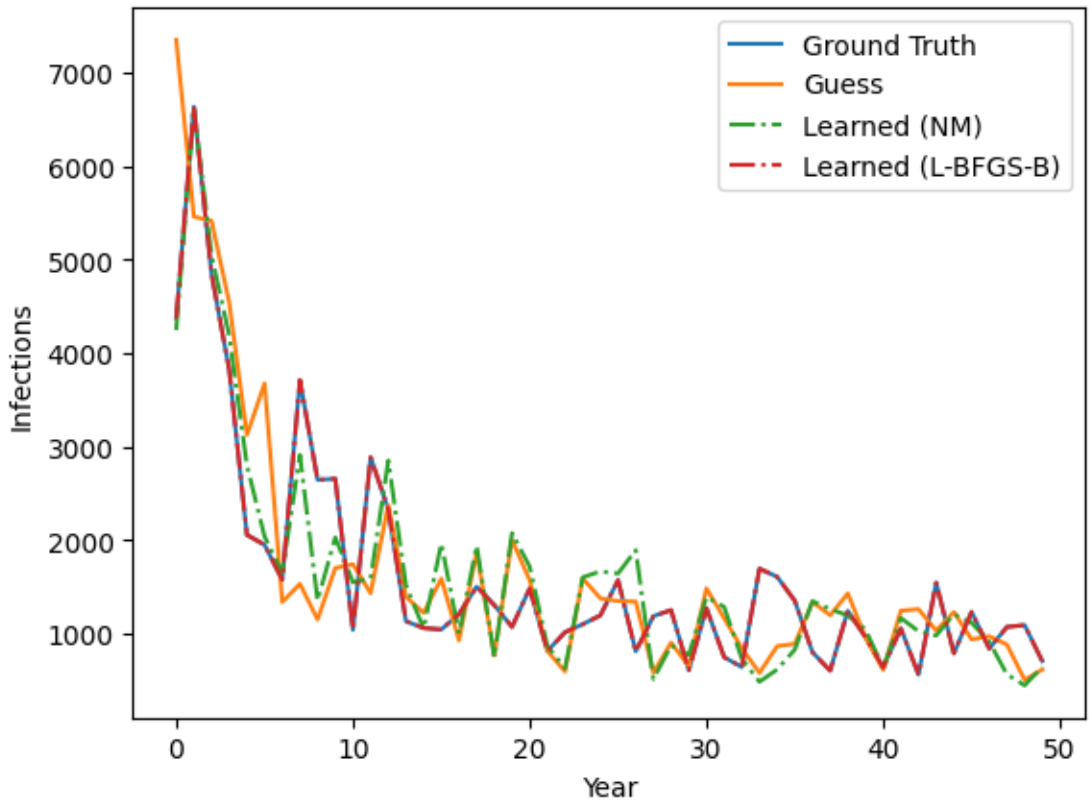
[6]:
```
initial_guess = np.random.uniform(0.05, 0.15, NUM_YEARS)
config_guess = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.YEAR,
    lambda_variation_params=initial_guess,
)
si_out_guess = catalytic_model(config_guess)
```

[7]:
```
results_nm = minimize(
    objective_function,
    x0=initial_guess,
    args=(LambdaVariationMethod.YEAR, si_out_gt,),
    method="Nelder-Mead",
    options={"maxiter": 1000},
)

results_bfgs = minimize(
    objective_function,
    x0=np.ones(NUM_YEARS) * 0.1,
    args=(LambdaVariationMethod.YEAR, si_out_gt,),
    method="L-BFGS-B",
    bounds=[(0.01, 0.25)] * NUM_YEARS,
    options={"maxiter": 100},
)
```

[8]:
```
config_nm = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.YEAR,
    lambda_variation_params=results_nm.x,
)
config_bfgs = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.YEAR,
    lambda_variation_params=results_bfgs.x,
```

```
)
nm_lambda_si_out = catalytic_model(config_nm)
bfgs_lambda_si_out = catalytic_model(config_bfgs)
```

[9]:
```
plt.plot(get_infections_by_year(si_out_gt), label="Ground Truth")
plt.plot(get_infections_by_year(si_out_guess), label="Guess")
plt.plot(get_infections_by_year(nm_lambda_si_out), '-.', label="Learned (NM)")
plt.plot(get_infections_by_year(bfgs_lambda_si_out), '-.', label="Learned␣
  ↪(L-BFGS-B)")
plt.ylabel("Infections")
plt.xlabel("Year")
plt.legend()
plt.show()
```



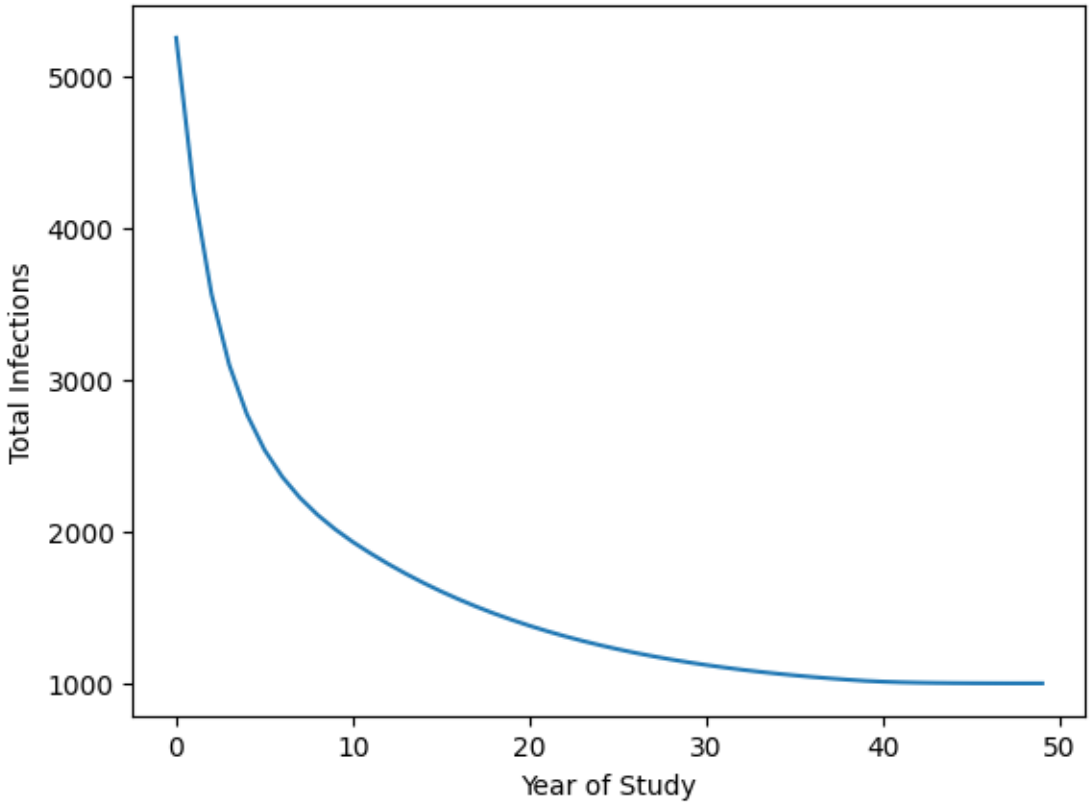
1.2 Variations HW 1

1.2.1 i) ii) iii) iv)

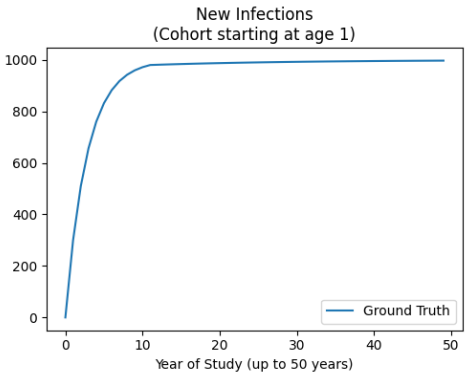
[10]:
```python
def plot_infections_by_age_cohort(
    si_out: np.ndarray,
    ages: list[int],
    is_ground_truth: bool = True,
    fig: Optional[plt.Figure] = None,
    axs: Optional[np.ndarray] = None,
) -> None:
    """
    Plot the infections by age cohort.

    :param si_out: Susceptible and Infected by age group and year
    :param ages: List of ages to plot
    :param is_ground_truth: If True, plot the ground truth
    :param fig: Figure to plot on
    :param axs: Axes to plot on

    :return: fig, axs
    """
    if not fig:
        fig_height = len(ages) * 16 // 4
        fig, axs = plt.subplots(len(ages), 2, figsize=(10, fig_height))

    ax = axs.flat

    if is_ground_truth:
        style = "-"
        label = "Ground Truth"
    else:
        style = "--"
        label = "Learned"
    # label = "Ground Truth" if is_ground_truth else "Learned"

    # Turn this is into a forloop where you pass in a value k to get the right␣
↪diagonal
    for i, age in enumerate(ages):
        susceptible_starting_at_age = np.diag(si_out[:, :, 0], k=age)
        infections_starting_at_age = np.diag(si_out[:, :, 1], k=age)

        ax[i*2].plot(infections_starting_at_age[:-1], label=label,␣
↪linestyle=style)
        ax[i*2].set_title(f"New Infections\n(Cohort starting at age {age + 1})")
        ax[i*2].set_xlabel("Year of Study (up to 50 years)")
        ax[i*2].legend()
```

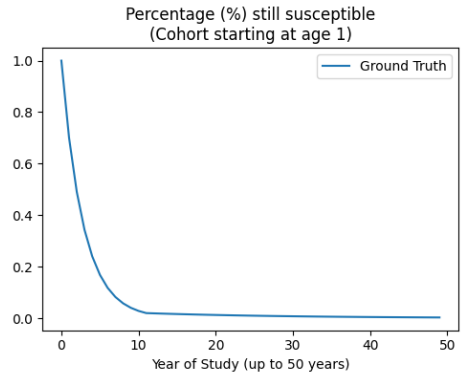
```
        ax[i*2 + 1].plot(susceptible_starting_at_age[:-1]/POPULATION_PER_AGE,␣
↪label=label, linestyle=style)
        ax[i*2 + 1].set_title(f"Percentage (%) still susceptible\n(Cohort␣
↪starting at age {age + 1})")
        ax[i*2 + 1].set_xlabel("Year of Study (up to 50 years)")
        ax[i*2 + 1].legend()

    plt.tight_layout()

    return fig, axs
```

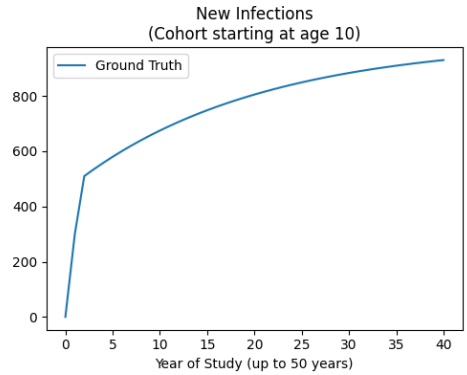
[11]:
```
config_foi_by_age_gt = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.AGE,
    lambda_variation_params=np.array([0.3, 0.05, 10]),
)
si_out_foi_by_age_gt = catalytic_model(config_foi_by_age_gt)

plt.plot(get_infections_by_year(si_out_foi_by_age_gt))
plt.ylabel("Total Infections")
plt.xlabel("Year of Study")
plt.show()
```

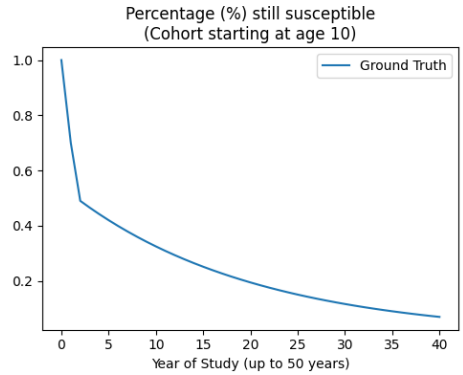


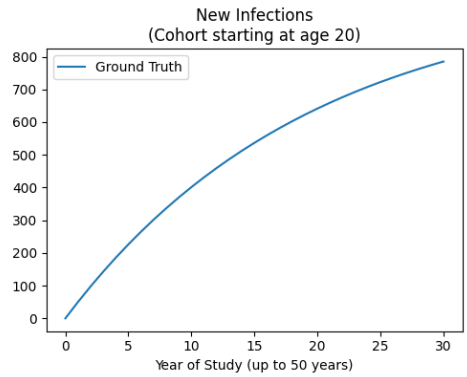
[12]:
```
fig, axs = plot_infections_by_age_cohort(
    si_out_foi_by_age_gt,
    ages=[0, 9, 19, 29, 39],
)
```

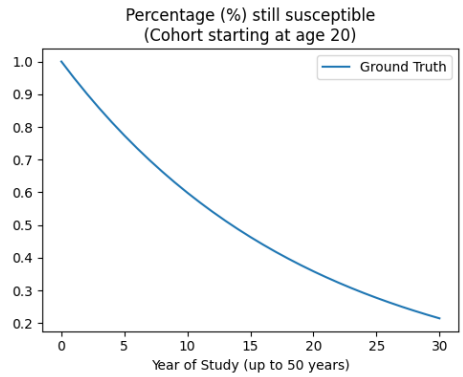

New Infections
(Cohort starting at age 1)
Ground Truth
Year of Study (up to 50 years)

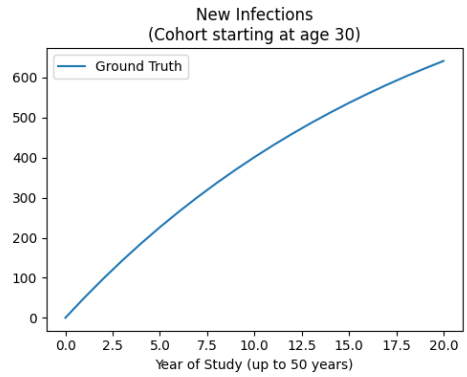

Percentage (%) still susceptible
(Cohort starting at age 1)
Ground Truth
Year of Study (up to 50 years)

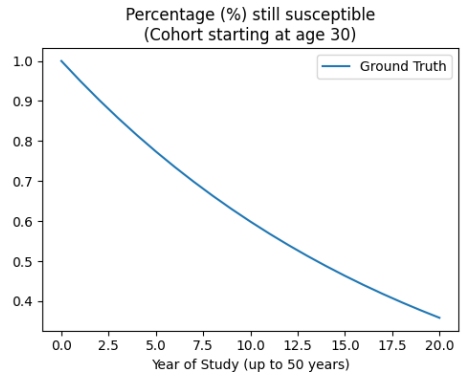

New Infections
(Cohort starting at age 10)
Ground Truth
Year of Study (up to 50 years)

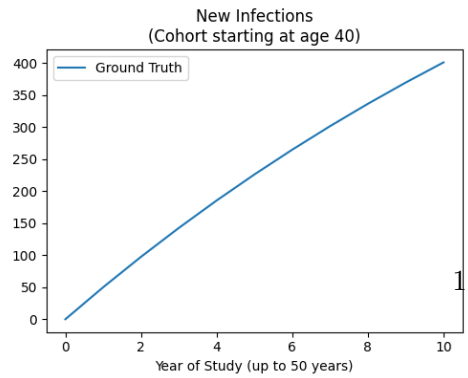

Percentage (%) still susceptible
(Cohort starting at age 10)
Ground Truth
Year of Study (up to 50 years)

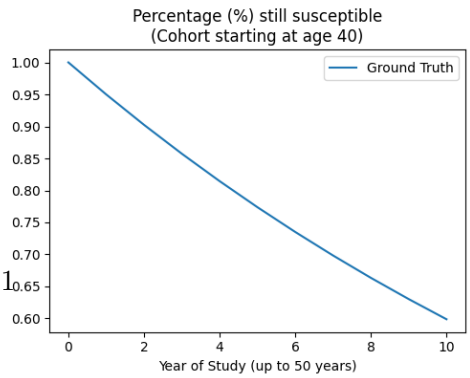

New Infections
(Cohort starting at age 20)
Ground Truth
Year of Study (up to 50 years)


Percentage (%) still susceptible
(Cohort starting at age 20)
Ground Truth
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 30)
Ground Truth
Year of Study (up to 50 years)


Percentage (%) still susceptible
(Cohort starting at age 30)
Ground Truth
Year of Study (up to 50 years)

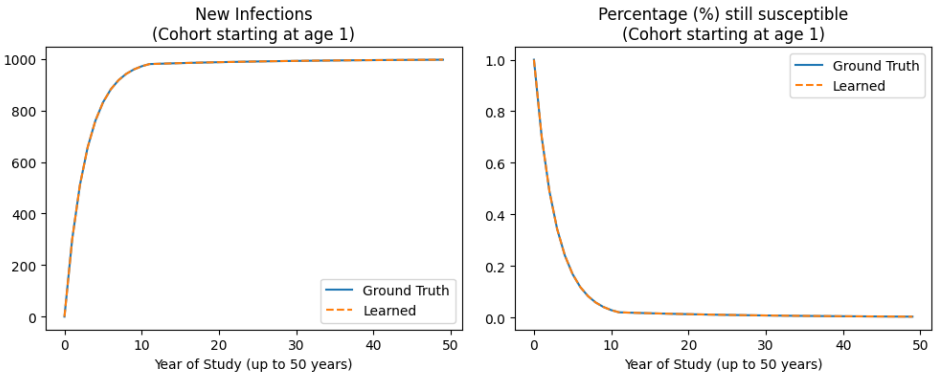

New Infections
(Cohort starting at age 40)
Ground Truth
Year of Study (up to 50 years)


Percentage (%) still susceptible
(Cohort starting at age 40)
Ground Truth
Year of Study (up to 50 years)

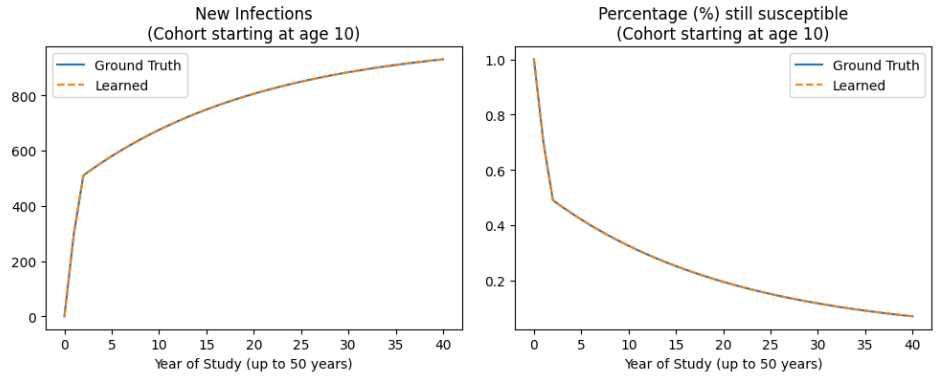
1.2.2 v)

[14]:
```
results_nm_lambda_by_age_partial = minimize(
    objective_function,
    x0=[0.1, 0.1],
    args=(LambdaVariationMethod.AGE, si_out_foi_by_age_gt, True, True, False),
    method="Nelder-Mead",
    options={"maxiter": 1000},
)
results_bfgs_lambda_by_age_partial = minimize(
    objective_function,
    x0=[0.1, 0.1],
    args=(LambdaVariationMethod.AGE, si_out_foi_by_age_gt, True, True, False),
    method="L-BFGS-B",
    bounds=[(0.01, 0.5), (0.01, 0.5)],
    options={"maxiter": 100},
)
config_bfgs_lambda_by_age_partial = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.AGE,
    lambda_variation_params=np.append(results_bfgs_lambda_by_age_partial.x, 10),
)
si_out_foi_by_age_partial_learned = ␣
 ↪catalytic_model(config_bfgs_lambda_by_age_partial)
```

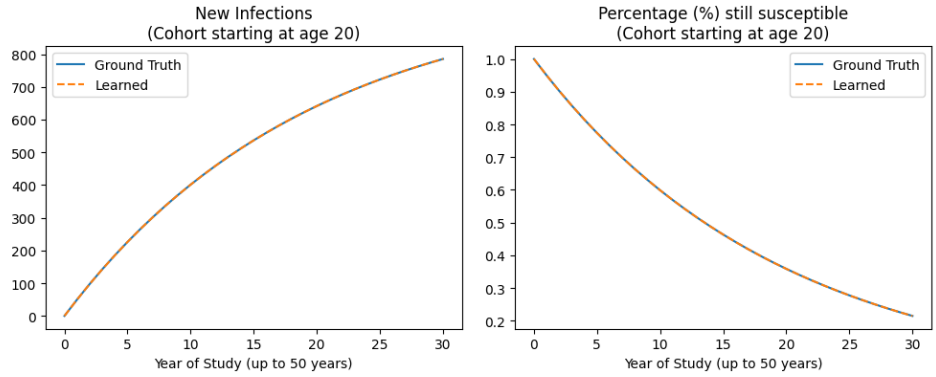
[15]:
```
ages = [0, 9, 19, 29, 39]

fig, axs = plot_infections_by_age_cohort(
    si_out_foi_by_age_gt,
    ages=ages,
)
fig, axs = plot_infections_by_age_cohort(
    si_out_foi_by_age_partial_learned,
    ages=ages,
    is_ground_truth=False,
    fig=fig,
    axs=axs,
)
plt.show()
```


New Infections
(Cohort starting at age 1)
Ground Truth
Learned
Year of Study (up to 50 years)

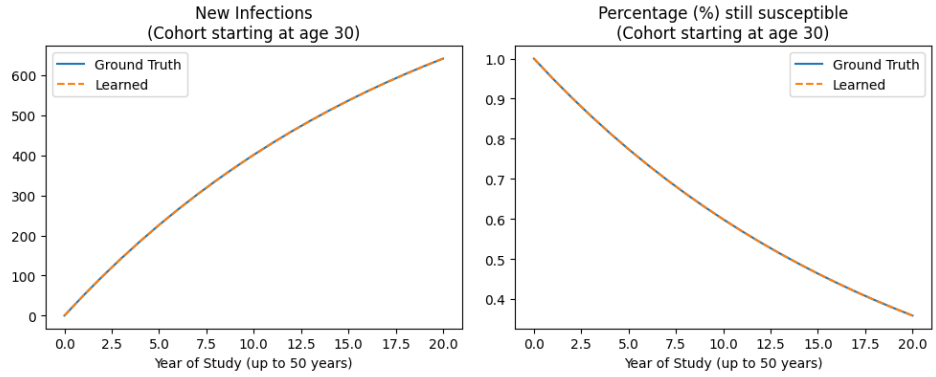
Percentage (%) still susceptible
(Cohort starting at age 1)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 10)
Ground Truth
Learned
Year of Study (up to 50 years)

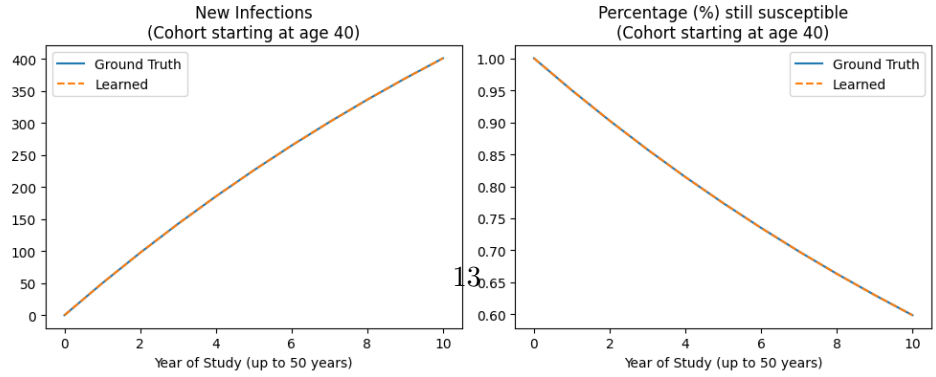
Percentage (%) still susceptible
(Cohort starting at age 10)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 20)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 20)
Ground Truth
Learned
Year of Study (up to 50 years)

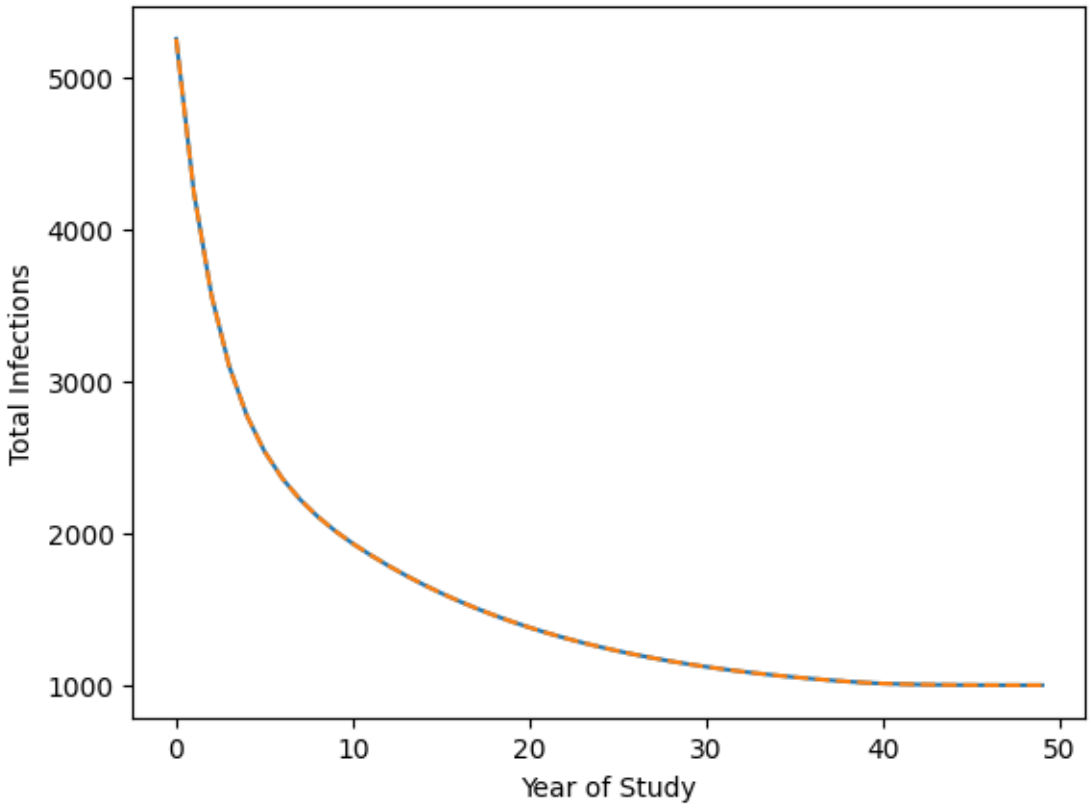

New Infections
(Cohort starting at age 30)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 30)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 40)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 40)
Ground Truth
Learned
Year of Study (up to 50 years)

[16]:
```
plt.plot(get_infections_by_year(si_out_foi_by_age_gt))
plt.plot(get_infections_by_year(si_out_foi_by_age_partial_learned),␣
 ↪linestyle="--")
plt.ylabel("Total Infections")
plt.xlabel("Year of Study")
plt.show()
```



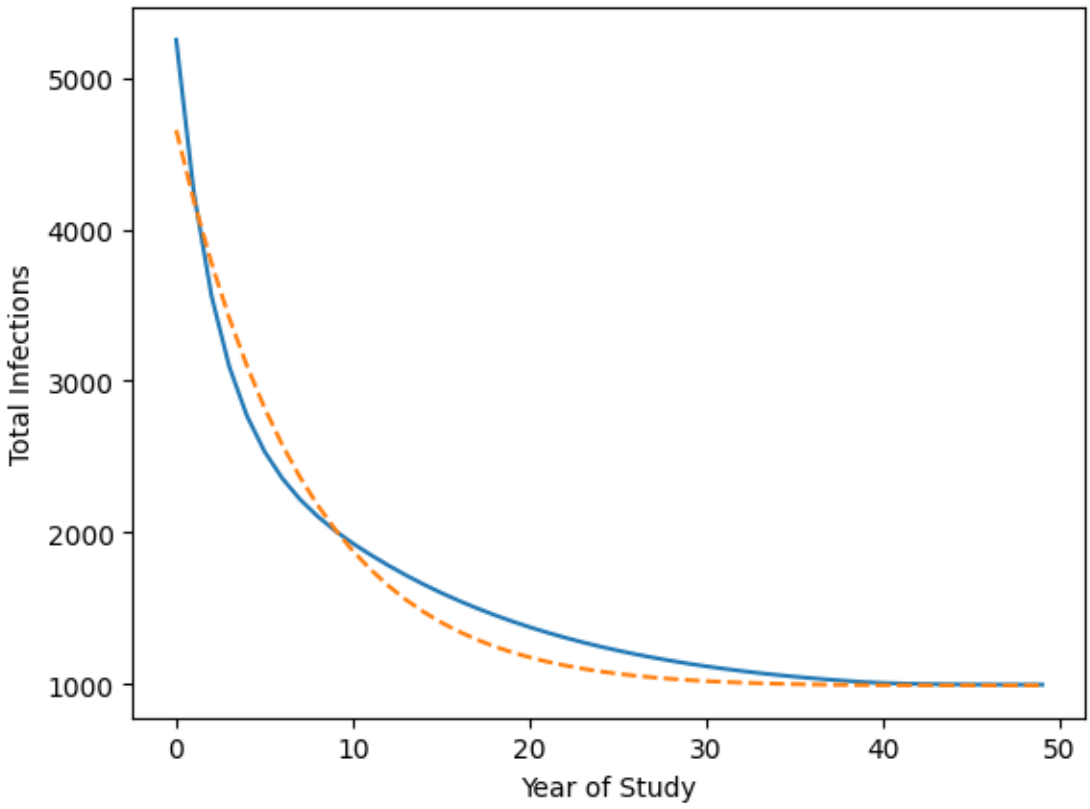
1.2.3 vi)

[17]:
```
results_nm_lambda_by_age_full = minimize(
    objective_function,
    x0=[0.1, 0.1, 5],
    args=(LambdaVariationMethod.AGE, si_out_foi_by_age_gt, True, True, True),
    method="Nelder-Mead",
    options={"maxiter": 1000},
)
results_bfgs_lambda_by_age_full = minimize(
    objective_function,
```

```
    x0=[0.1, 0.1, 5],
    args=(LambdaVariationMethod.AGE, si_out_foi_by_age_gt, True, True, True),
    method="L-BFGS-B",
    bounds=[(0.01, 0.5), (0.01, 0.5), (0, 50)],
    options={"maxiter": 100},
)
```

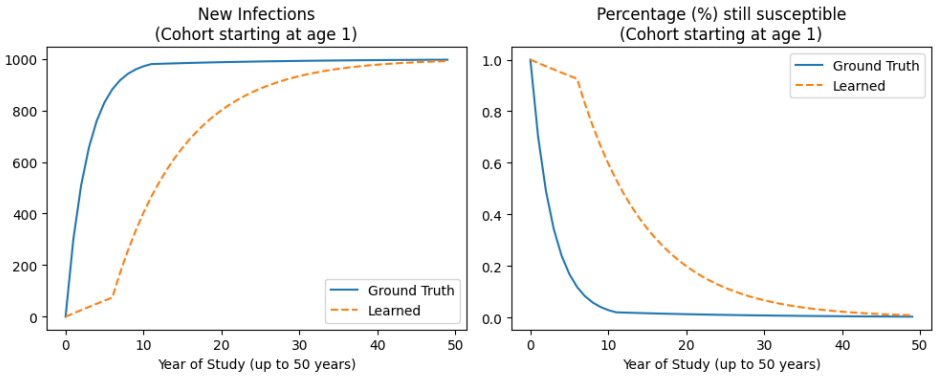
[18]:
```
config_bfgs_lambda_by_age_full = prepare_catalytic_model_config(
    lambda_variation_method=LambdaVariationMethod.AGE,
    lambda_variation_params=results_bfgs_lambda_by_age_full.x,
)
si_out_foi_by_age_full_learned = catalytic_model(config_bfgs_lambda_by_age_full)
```

[19]:
```
plt.plot(get_infections_by_year(si_out_foi_by_age_gt))
plt.plot(get_infections_by_year(si_out_foi_by_age_full_learned), linestyle="--")
plt.ylabel("Total Infections")
plt.xlabel("Year of Study")
plt.show()
```

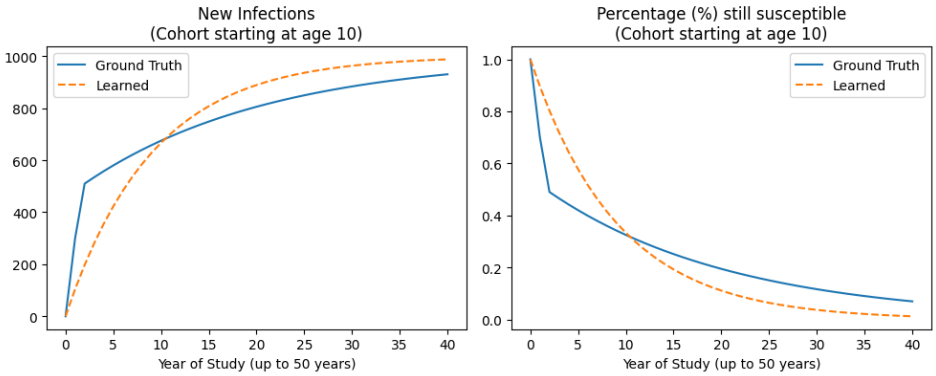


[20]:
```
fig, axs = plot_infections_by_age_cohort(
    si_out_foi_by_age_gt,
```

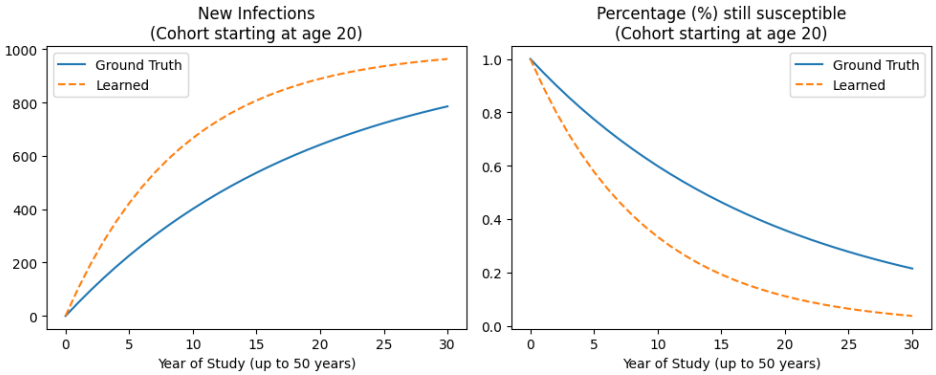
```
    ages=ages,
)
fig, axs = plot_infections_by_age_cohort(
    si_out_foi_by_age_full_learned,
    ages=ages,
    is_ground_truth=False,
    fig=fig,
    axs=axs,
)
plt.show()
```


New Infections
(Cohort starting at age 1)
Ground Truth
Learned
Year of Study (up to 50 years)

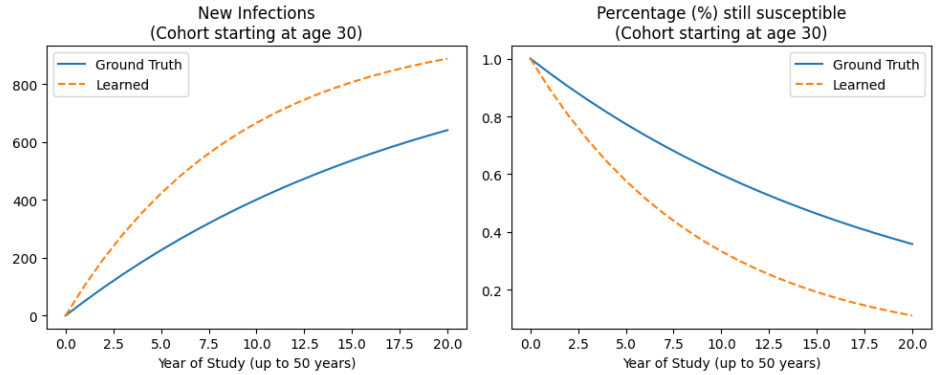
Percentage (%) still susceptible
(Cohort starting at age 1)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 10)
Ground Truth
Learned
Year of Study (up to 50 years)

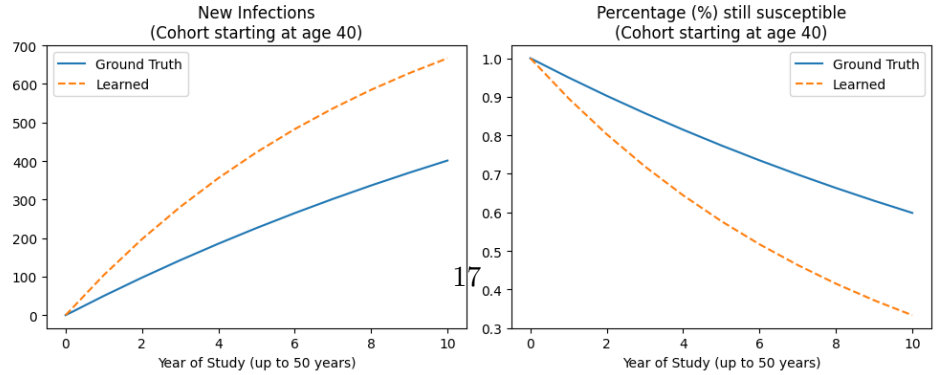
Percentage (%) still susceptible
(Cohort starting at age 10)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 20)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 20)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 30)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 30)
Ground Truth
Learned
Year of Study (up to 50 years)


New Infections
(Cohort starting at age 40)
Ground Truth
Learned
Year of Study (up to 50 years)

Percentage (%) still susceptible
(Cohort starting at age 40)
Ground Truth
Learned
Year of Study (up to 50 years)

[ ]: