Lecture 3: Inductive bias, regularization, and ensemble methods

Stefan Bucher

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Open in Colab

Prince (2023, chaps. 5, 9); Murphy (2022, chap. 18).[1]

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Generalization and inductive bias

- **Generalization:** performance on unseen (test) data
- **Inductive bias:** assumptions that favour some solutions over others (e.g. smoothness, sparsity); determines model behavior in underdetermined regimes and hence generalization.
- Today: concrete tools to improve generalization.

Outline

1. **Regularization** — constrain or perturb parametric models (L2, L1, dropout, transfer, etc.).
2. **Nonparametric methods** — Classification and Regression Trees (CART).
3. **Ensemble methods** — Bagging, random forests, boosting, XGBoost.
4. **Interpretability** — Shapley values and SHAP for feature attribution.
5. **Prediction vs. inference**

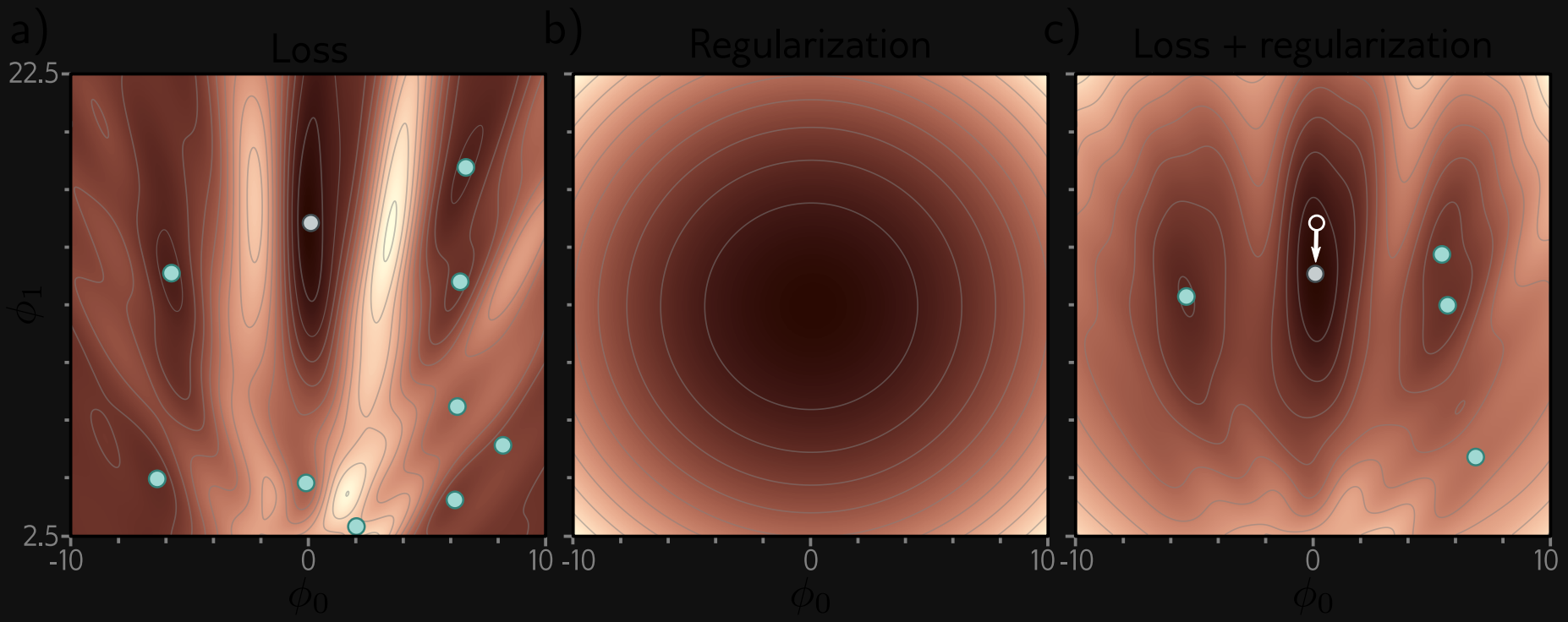
Regularization

Goal: Reduce generalization gap between training and test performance.

Prince (2023, chap. 9)

Explicit Regularization

$$\hat{\phi} = \underset{\phi}{\arg\min} \sum_{i=1}^{I} l_i[x_i, y_i] + \lambda g[\phi]$$



Interpretation as Bayesian Prior

Maximum a posteriori (MAP) instead of maximum LLH

$$\hat{\phi} = \arg\max_{\phi} \prod_{i=1}^{I} q(y_i|\theta_i = f[x_i, \phi])P(\phi)$$

$$= \arg\max_{\phi} \log \prod_{i=1}^{I} q(y_i|\theta_i = f[x_i, \phi])P(\phi)$$

$$= \arg\min_{\phi} -\log P(\phi) - \sum_{i=1}^{I} \log q(y_i|\theta_i = f[x_i, \phi])$$

$$= \arg\min_{\phi} \lambda g[\phi] + \sum_{i=1}^{I} l_i[x_i, y_i]$$

L2 regularization: Ridge regression

$$g[\phi] = \sum_j \phi_j^2$$

L1 regularization: Lasso regression

$$g[\phi] = \sum_j |\phi_j|$$

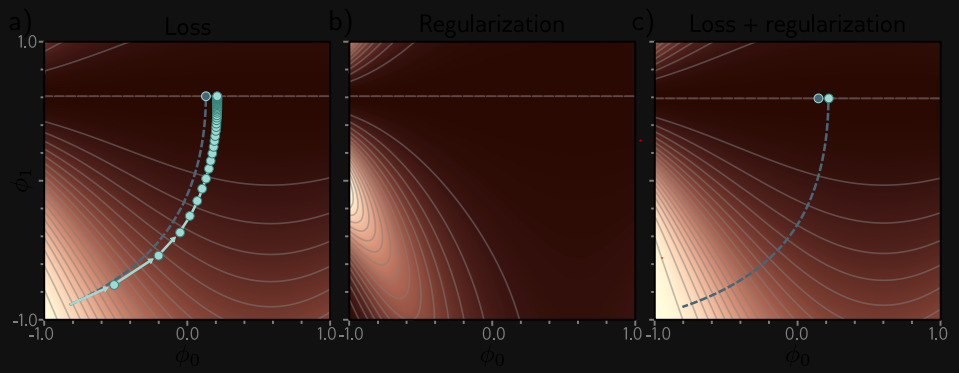
Implicit Regularization

Discrete stochastic gradient descent on L arrives at same place as continuous descent $\frac{d\phi}{dt} = -\frac{\partial \tilde{L}}{\partial \phi}$ on

$$\tilde{L}[\phi] = L[\phi] + \frac{\alpha}{4}||\frac{\partial L}{\partial \phi}||^2 + \frac{\alpha}{4B}\sum_{b=1}^{B}||\frac{\partial L_b}{\partial \phi} - \frac{\partial L}{\partial \phi}||^2$$

so is naturally biased

- away from steep gradients
- to stable gradients (low variance across batches), suggesting that “all data fits well” and promising better generalization

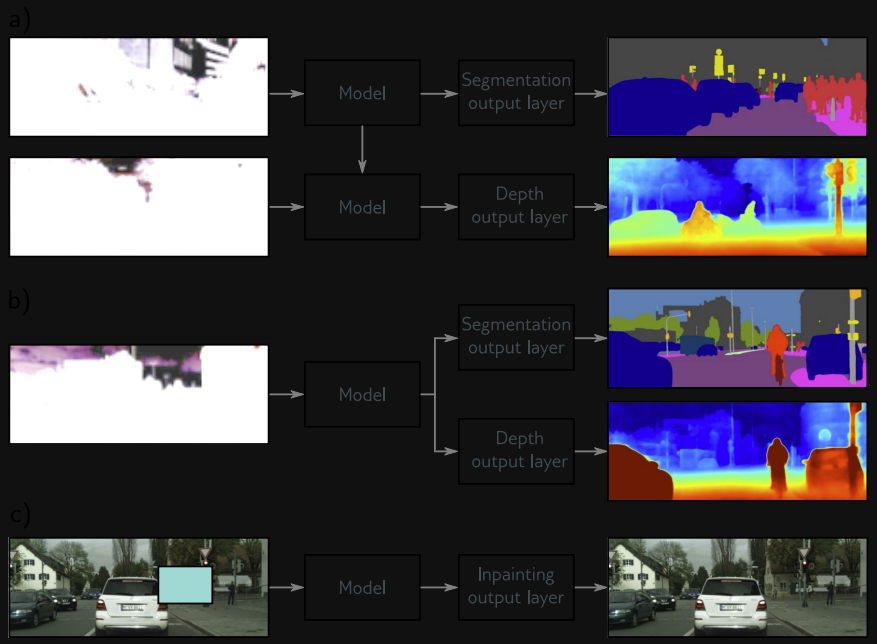


Performance Heuristics

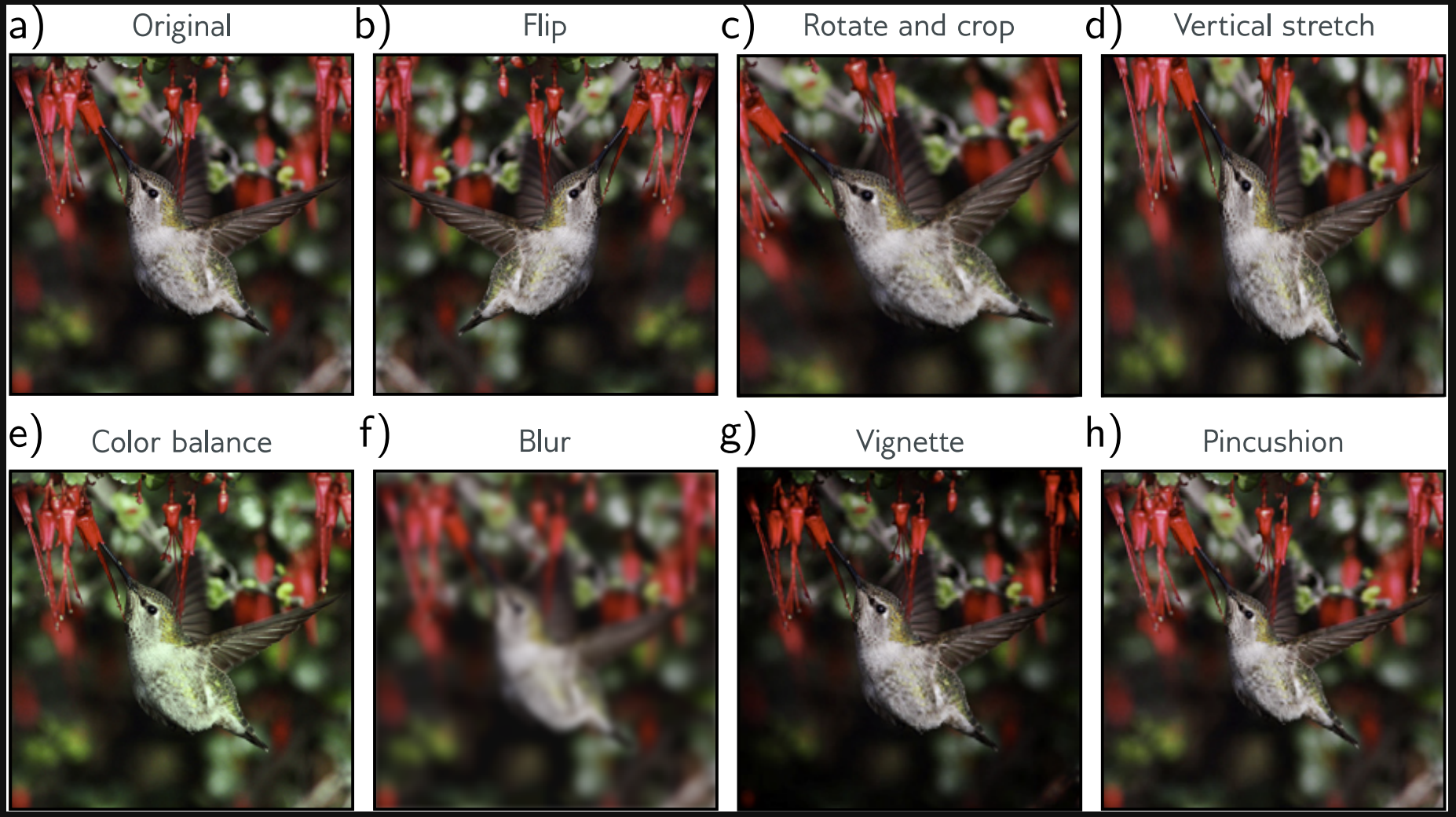
- **Early stopping:** halt training when validation loss starts rising; avoids overfitting by limiting effective model complexity w/o changing architecture.
- **Noise injection:** add noise to inputs, weights, or labels during training; acts as a smoothing penalty and improves robustness
  - adversarial training is a targeted variant
- **Normalization** (batch, layer, group): re-center and re-scale activations within each layer; stabilizes and accelerates training by reducing internal covariate shift
- **Bayesian inference:** instead of point estimates of the parameters, consider posterior $P(\phi|\{x_i, y_i\}) \propto \prod_{i=1}^{I} q(y_i|x_i, \phi)P(\phi)$
  - principled but often intractable

Transfer & Self-supervised Learning

- Transfer learning (pretrain on related training data)
  - train final layers
  - fine-tune whole model
- Multi-task learning
- Self-supervised learning
  - generative (fill in masked data)
  - contrastive (compare pairs of examples for relatedness)

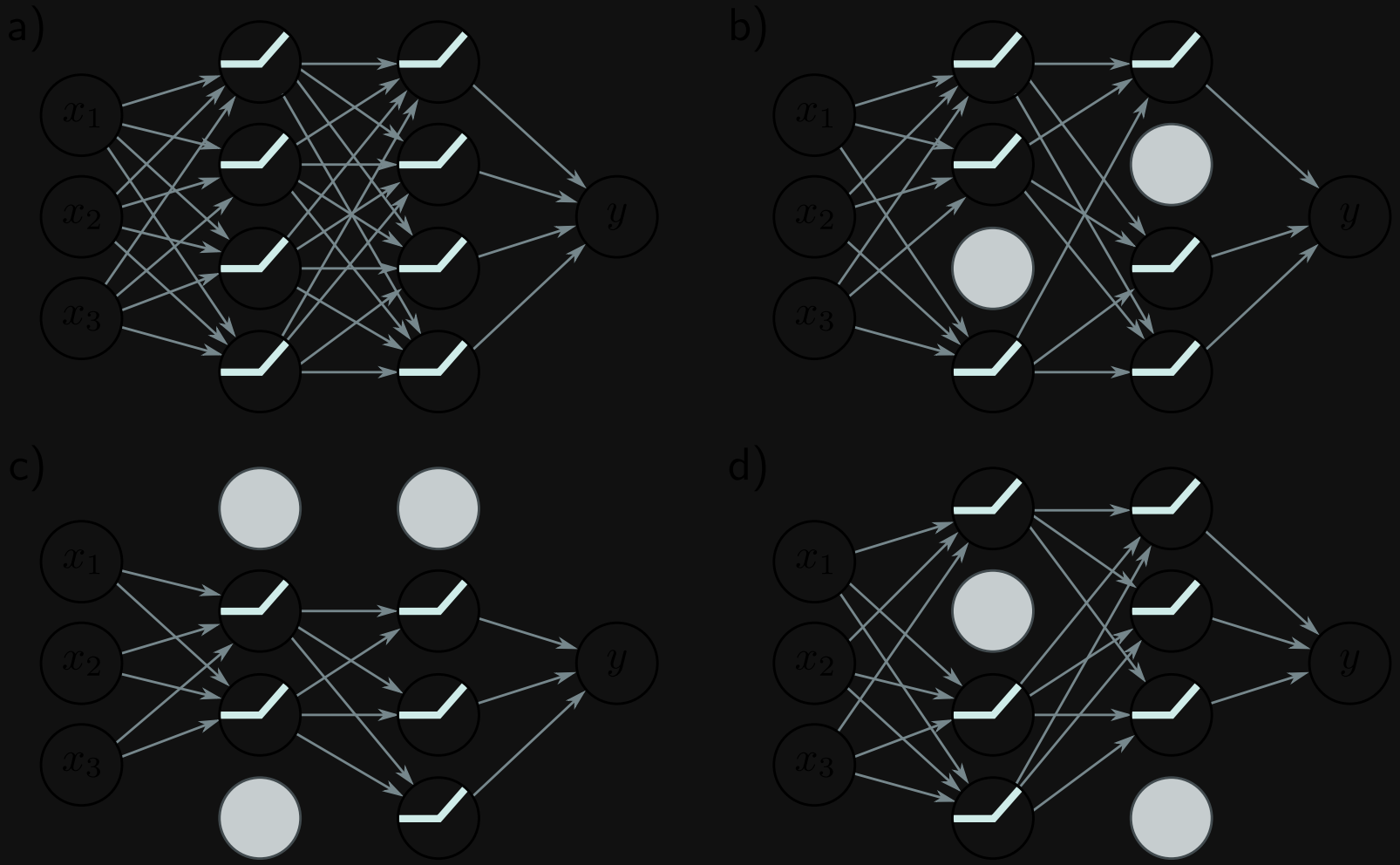


Data Augmentation

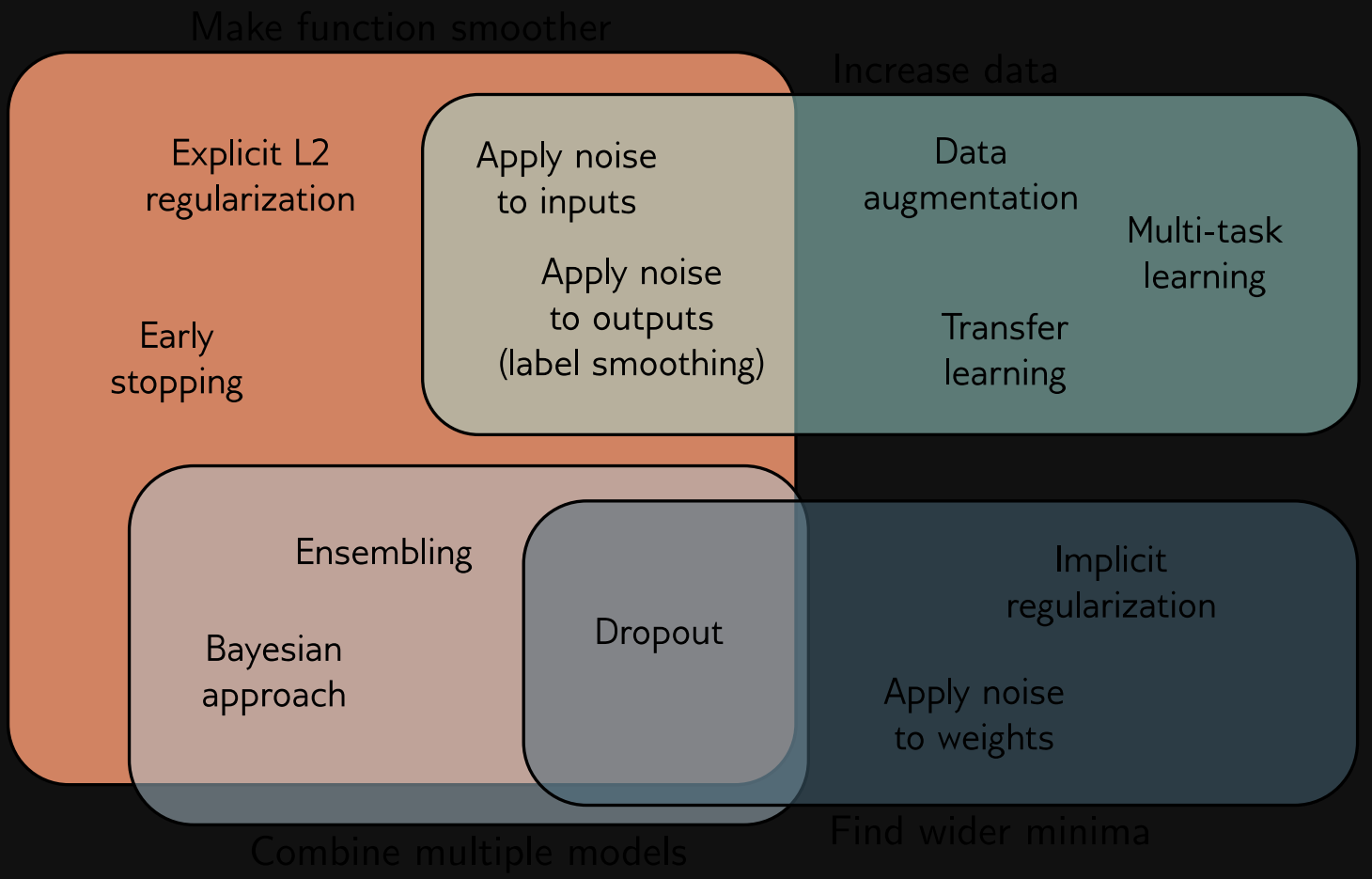


Dropout

Clamping subset of hidden units to zero.



Regularization Overview



Ensemble methods

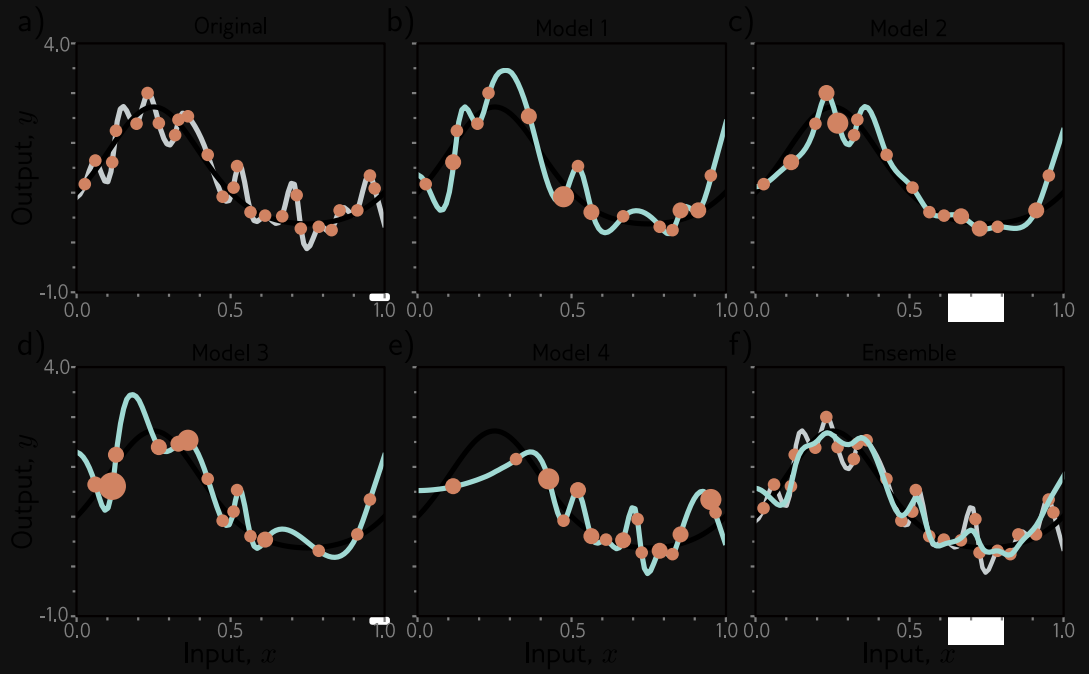
Murphy (2022, chaps. 18.2–18.5)

Explained through decision trees; ideas apply more generally.

Ensemble Methods

Average predictions of multiple models, e.g.

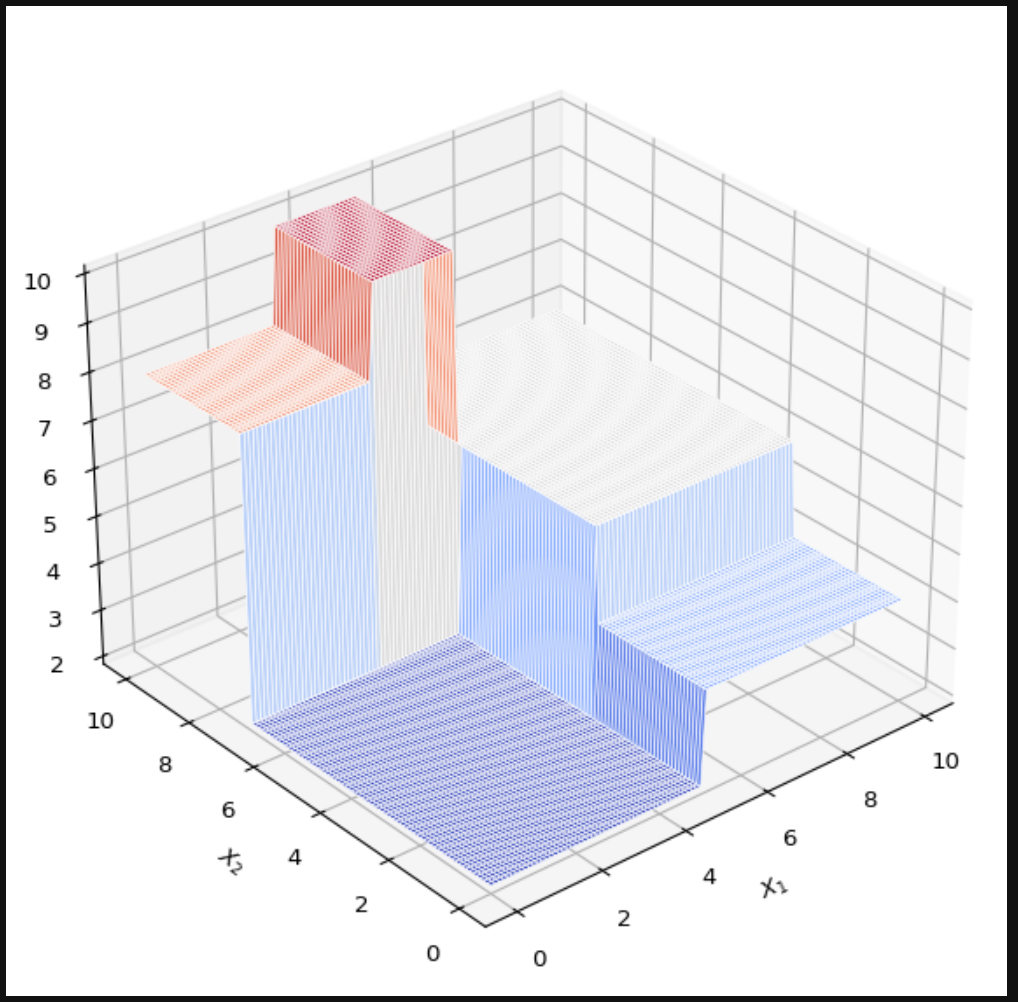
- different initializations
- Bagging (bootstrap aggregating)
  - i.e. resampling training data



CART: Classification and Regression Trees

Cf. D300 & Murphy (2022, chap. 18.1).

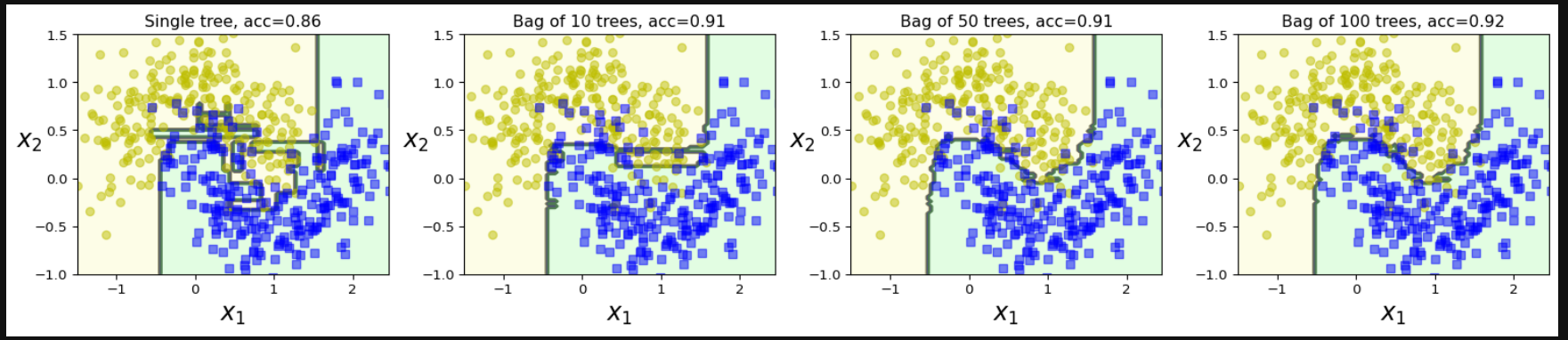
- Recursive axis-parallel splits: choose feature + threshold to minimize impurity
  - regression: MSE
  - classification: entropy or Gini index
- Partitions input space into (axis-aligned) regions of constant prediction.



Adapted from Murphy (2022, fig. 18.1).

Bagging: Bootstrap aggregating

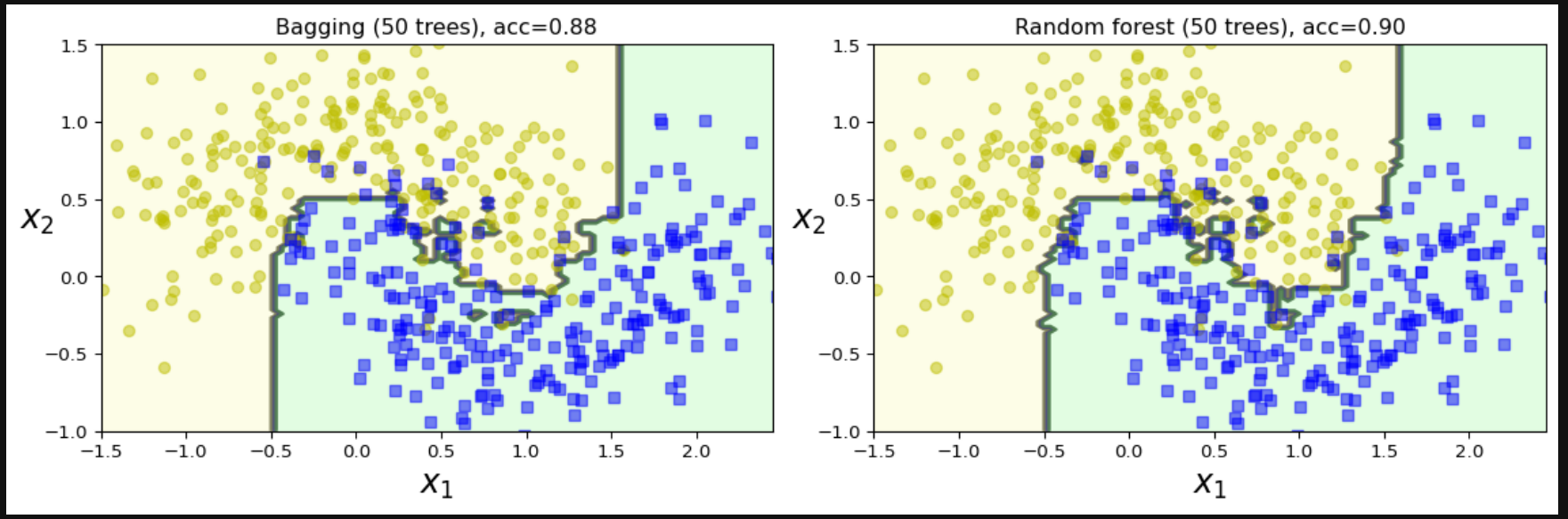
- Trees interpretable, but high variance (sensitive to data).
- **Bootstrap aggregating:** fit many models in parallel on bootstrap samples of the training data; average their predictions.
- Averaging (or voting) reduces variance.



Adapted from Murphy (2022, fig. 18.4).

Random forests

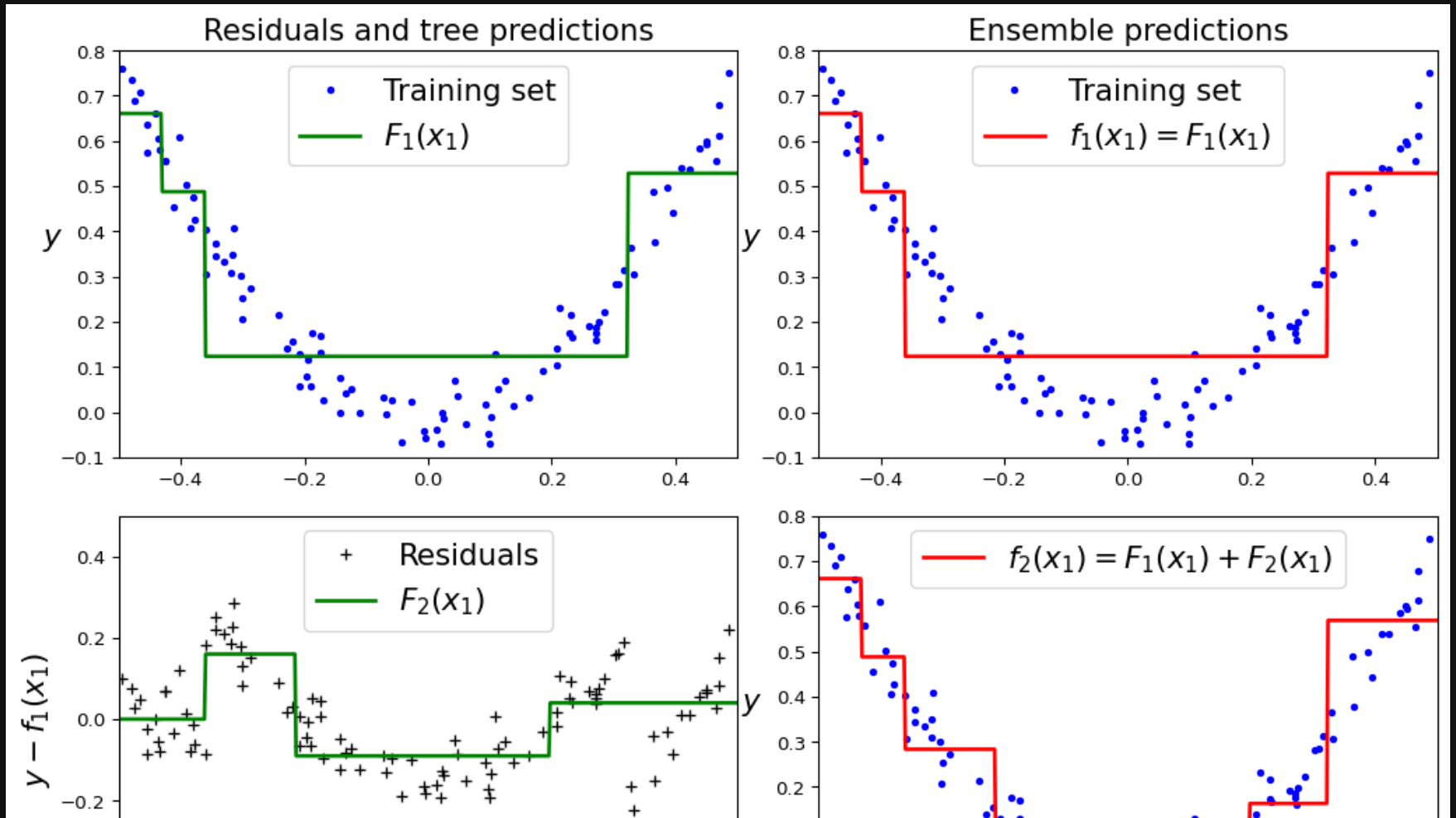
- Bagging but at each split use a random subset of features.
- Further decorrelates trees.

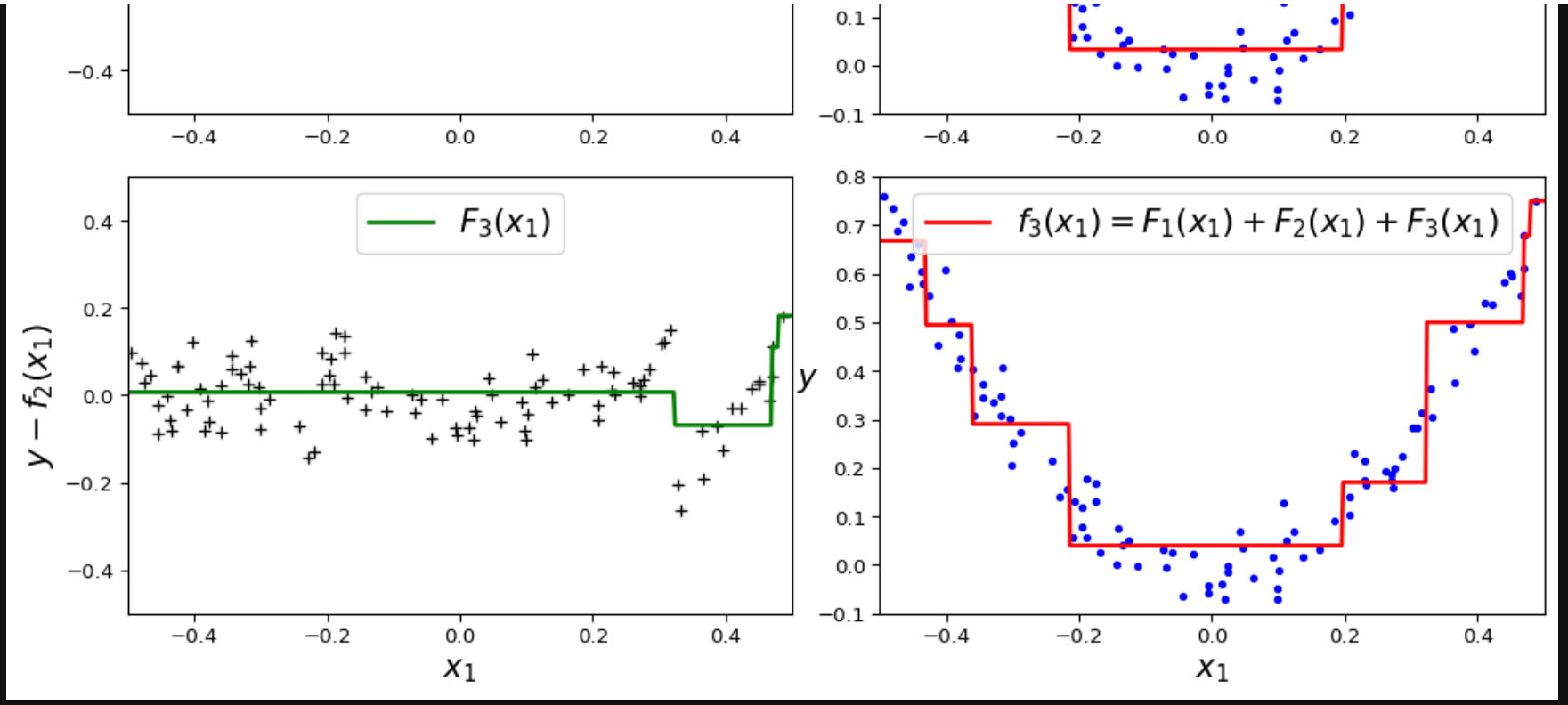


Adapted from Murphy (2022, fig. 18.4).

Boosting

Sequential: each new model focuses on errors (residuals) of the previous ones to iteratively improve weak learners.





Adapted from Murphy (2022, fig. 18.6).

Gradient Boosting and XGBoost

- **Gradient boosting:** sequentially fit shallow trees to the negative gradient (pseudo-residuals) of the loss.
  - Gradient descent in function space: each step adds a small tree pointing in the direction that most reduces prediction error.
- **XGBoost:** efficient implementation that adds L2 regularization on leaf weights, second-order (Newton) splits, column subsampling, and efficient handling of sparse data.
  - State-of-the-art for tabular data.

Model interpretability

Feature attribution

Question:
> *Which input features contributed to this model prediction?*

Core idea - Decompose a prediction into **additive feature contributions** - Explain the **model's behavior**, not the data-generating process

Typical output - Baseline prediction
- + contribution of feature 1
- + contribution of feature 2
- ... = final prediction

What it is good for - Debugging models
- Auditing decisions
- Communicating model logic at a high level

Shapley Values and SHAP

- **Shapley value:** feature j's average marginal contribution over all feature subsets (cooperative game theory)
- **SHAP:** efficient approximation; treats features as players, prediction as payoff.
- Uniquely satisfies efficiency, symmetry, and consistency.