Geostatistical data

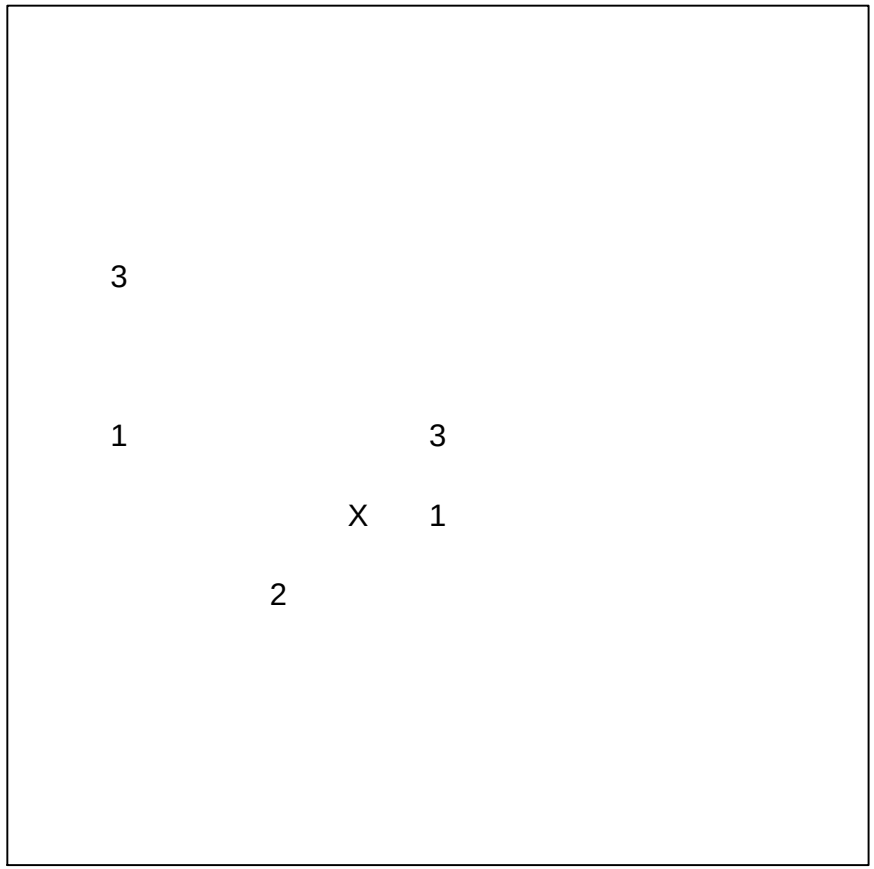
- Quantity measured at a location
  - Assumed characteristic of that location, not a large area
  - Examples:
    elevation, annual rainfall, surface soil pH, O_2 concentration at 3m
- Notation:
  - $\boldsymbol{s}$: location, a vector value.
    - Usually $\boldsymbol{s} = (x, y)$ in some coordinate frame (e.g., longlat or UTM)
    - Written as a vector because details of 1D (beach, line), 2D (earth surface), 3D (ocean, soil, atmosphere) not important
  - $Z(\boldsymbol{s})$: the characteristic at location $\boldsymbol{s}$.
- Geostatistical data
  - $Z(\boldsymbol{s})$ exists everywhere within boundary of study area
  - Generally, no sharp changes (jumps) in $Z(\boldsymbol{s})$
  - $Z(\boldsymbol{s}_1)$ probably different from $Z(\boldsymbol{s}_2)$, but transition is smooth

Many possible goals

- Predict $Z(\boldsymbol{s})$ at unmeasured locations
- Describe spatial pattern in $Z(\boldsymbol{s})$
  - How similar is $Z(\boldsymbol{s})$ to neighboring values?
  - How does that change with distance to neighbor?
- Model relationship between $Z(\boldsymbol{s})$ and covariates

Prediction

- Could be done to fill in a grid so can draw map or use image/contour plot
- Or, done because you need predictions at unmeasured points



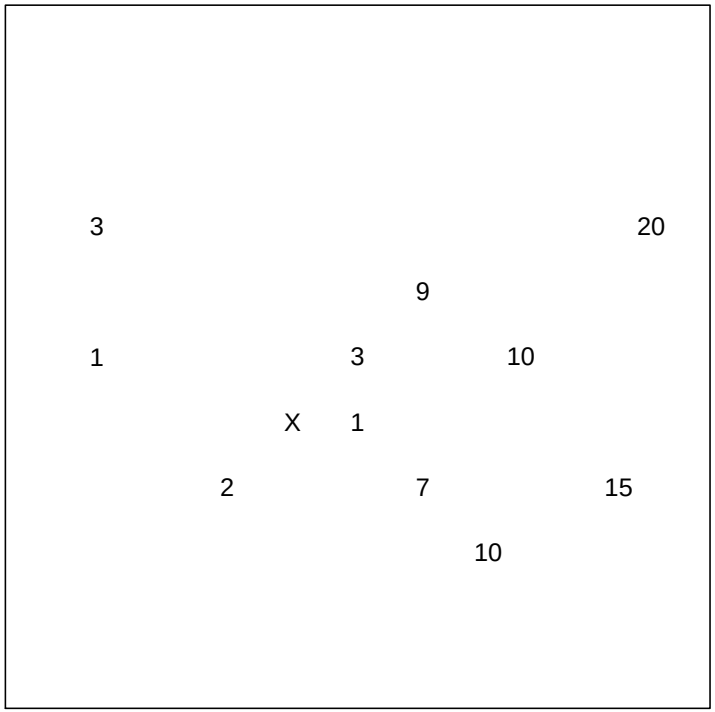
- What is Z at the location marked by X?

Prediction

- One possibility: simple average of Z over entire region
  - Very common in non-spatial contexts
- 1st law of geography (Tobler): everything is related to everything else more closely related to nearby things
- This principle is very important if there is a spatial trend (variation across the region) or some form of spatial pattern.
  - simple average ignores spatial trend and pattern

Prediction

- What if had a bit more data:



- Overall average for region clearly inappropriate
- Consider some form of local average
- We will discuss 3 methods:
  - Inverse distance weighting
  - Spatial trend model
  - Kriging: we'll spend most time / effort on this

Inverse distance weighting

- Concept:
  - Prediction an average that emphasizes nearby values
  - Done by weighting all observations
  - Higher weight to nearby observations
- Notation: $\boldsymbol{s}_i$ is location of i'th observation
  d_{ij} is distance between location i and location j
  $Z(\boldsymbol{s}_i)$ is value of Z at location $\boldsymbol{s}_i$
  $\hat{Z}(\boldsymbol{s}_i)$ is prediction of Z at location $\boldsymbol{s}_i$

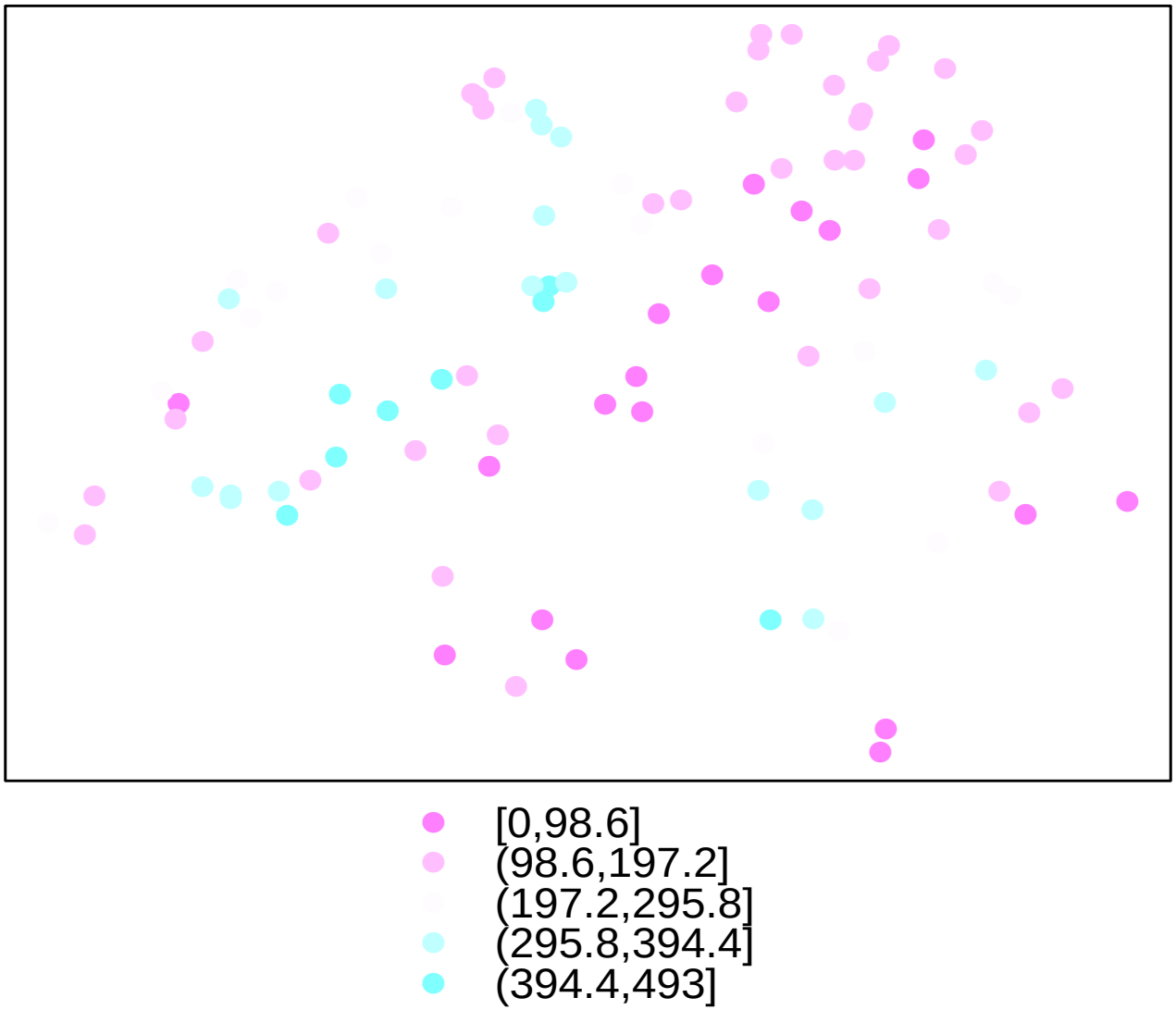
$$\hat{Z}(\boldsymbol{s}_j) = \frac{\sum_i w_{ij} Z(\boldsymbol{s}_i)}{\sum_i w_{ij}}, \text{where}$$

$$w_{ij} = \frac{1}{d_{ij}^a}$$

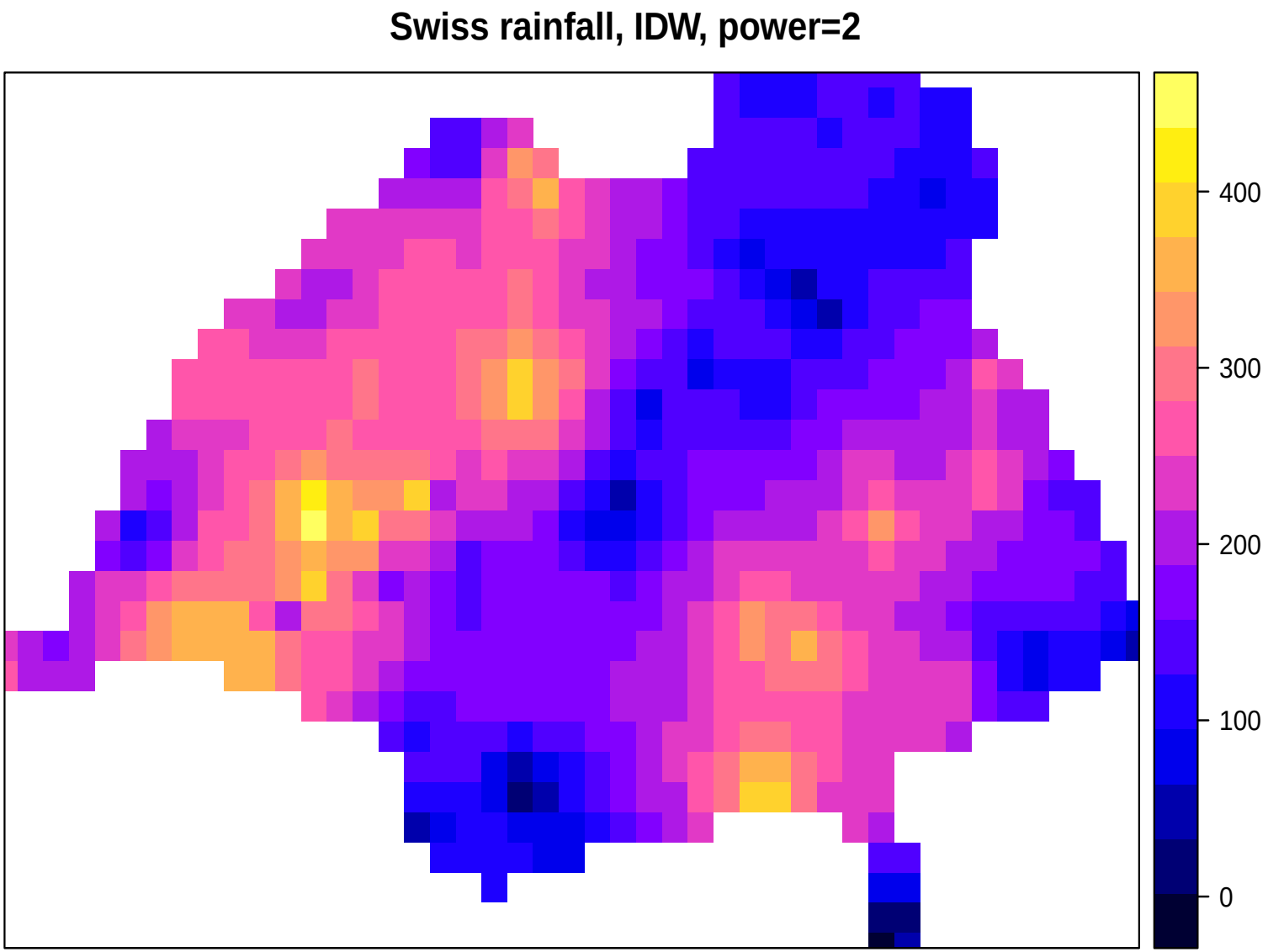
Inverse distance weighting

- a is an arbitrary parameter, commonly 1 or 2
  - $a = 0$ gives you the simple average over entire region (all weights $= 1$)
  - larger values $\rightarrow$ "more local" estimate, because emphasize shorter distances
  - if $d_{ij} = 0$, i.e. predicting at an observed location, use observed value
- Characteristics:
  - w_{ij} always ≥ 0 and w_{ij}/sum always ≤ 1
  - Sometimes set small values of w_{ij} to 0
  - $\hat{Z}(\boldsymbol{s}_j)$ always within range of observed values
    Some like this; other's don't.
- Problem: have to choose a. Some approaches:
  - Ad hoc (you like the resulting picture),
  - or tradition (your field always uses 2 or 1.5 or ??)
- demonstrate role of a by comparing results for $a = 2$ and $a = 1$

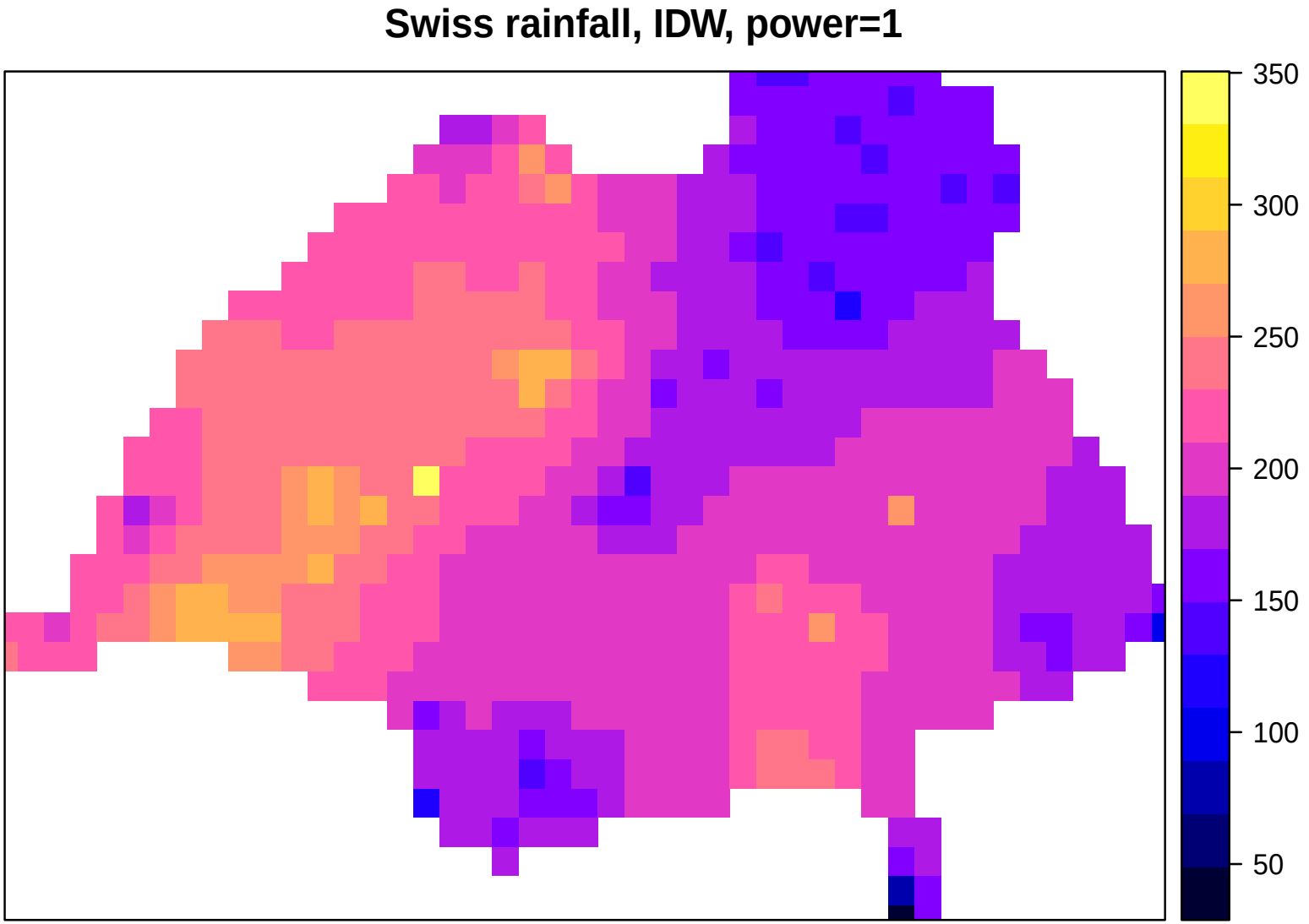
Swiss rainfall data



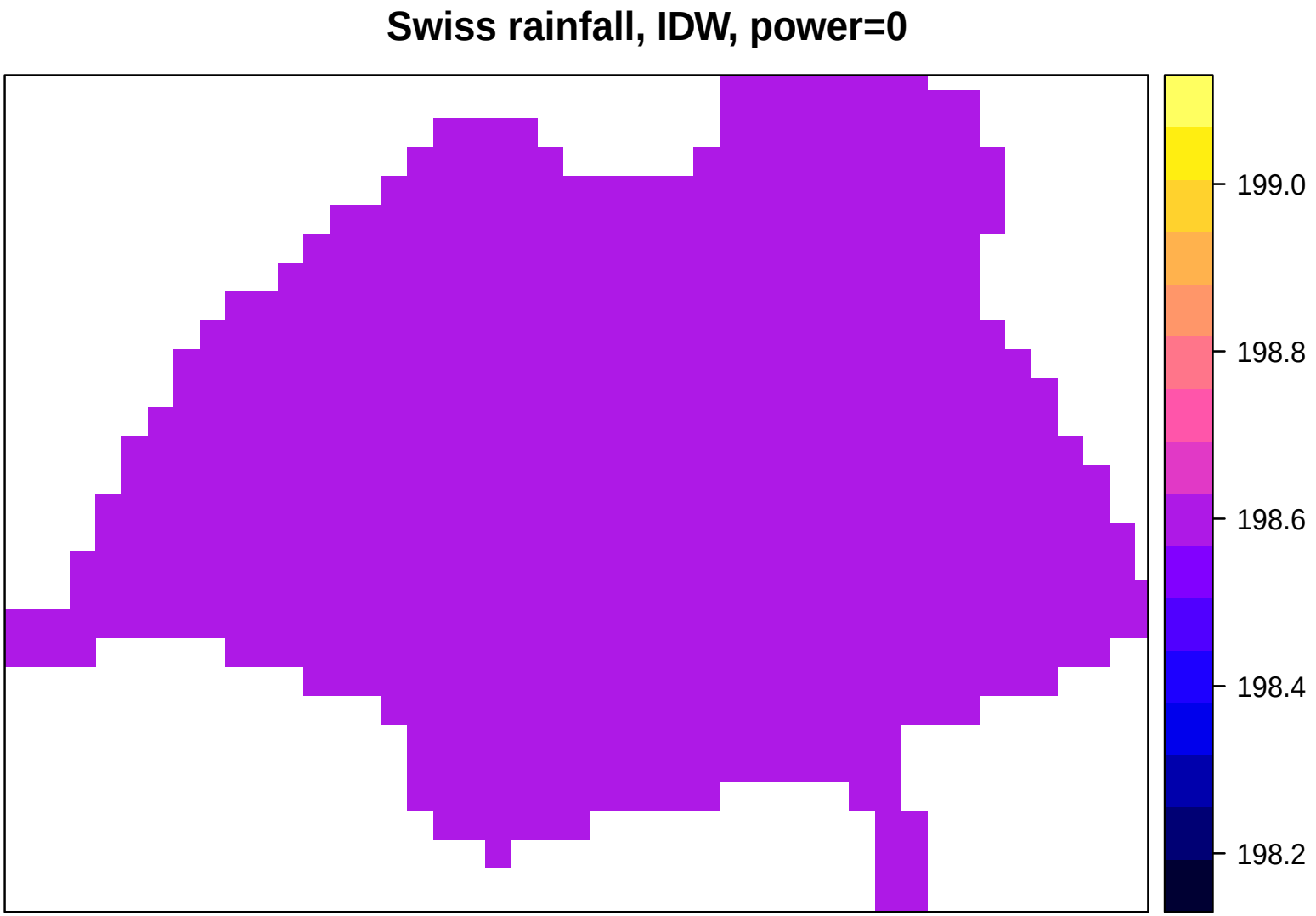
Swiss rain, IDW, power=2



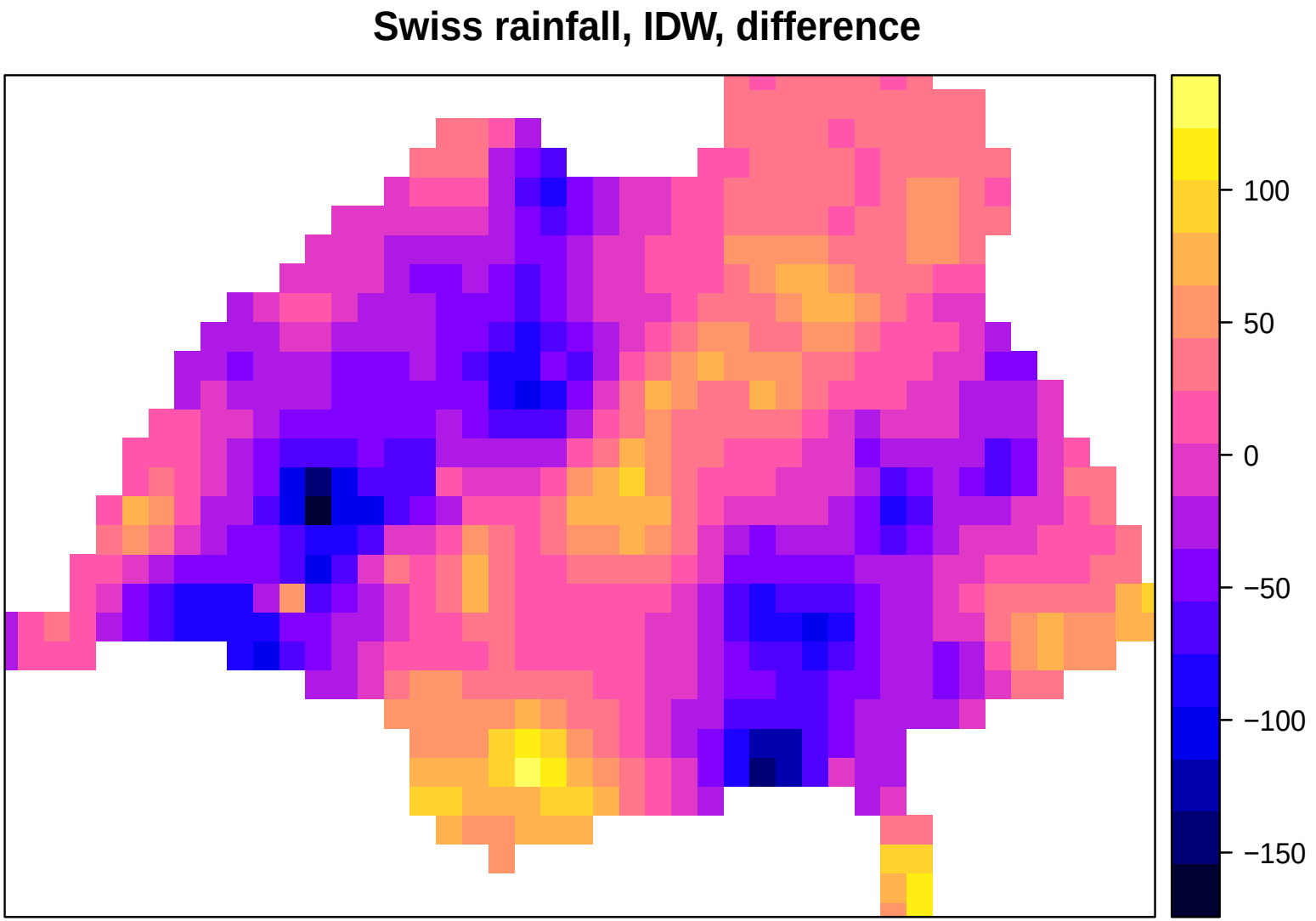
Swiss rain, IDW, power=1



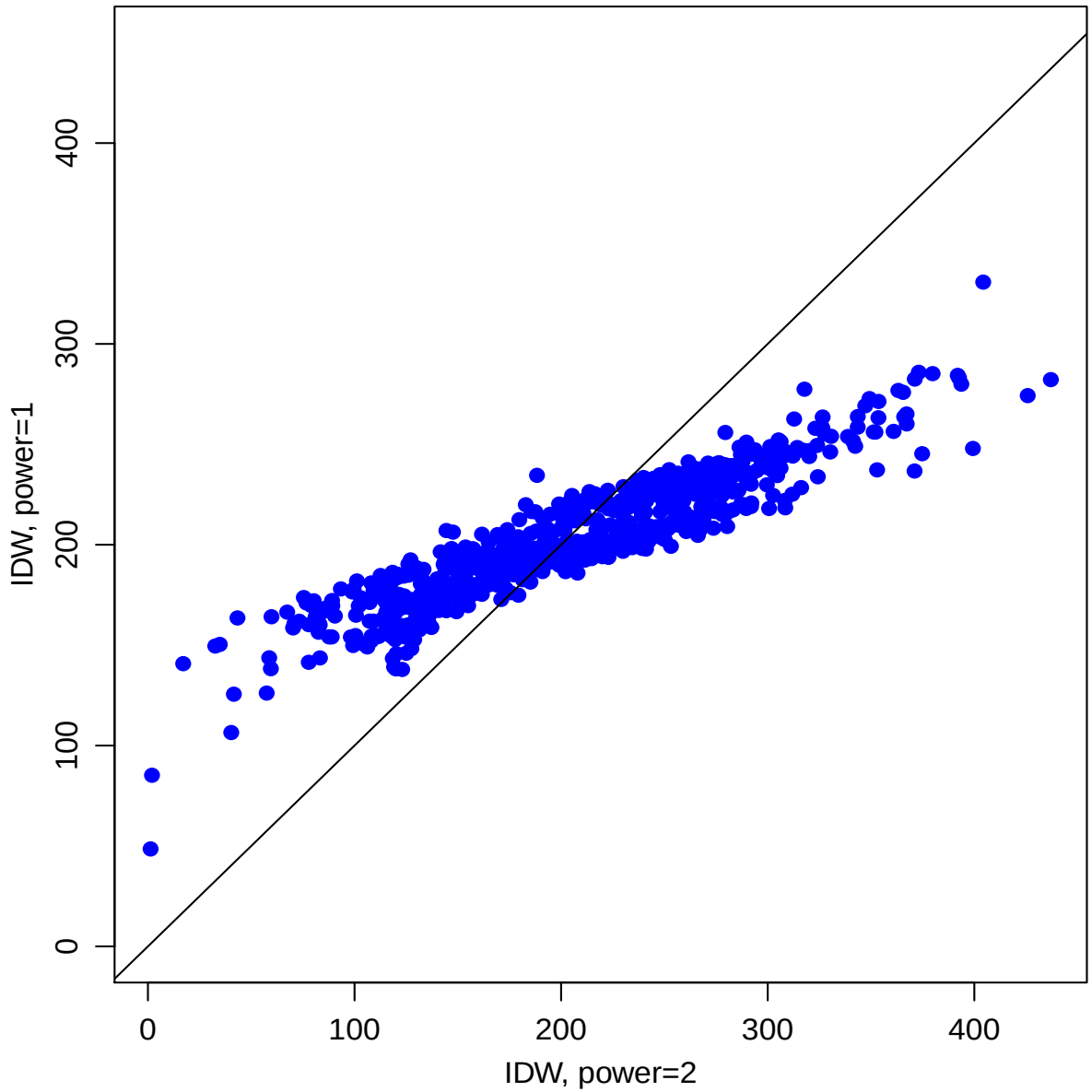
Swiss rain, IDW, power=0



Swiss rain, IDW, difference



Swiss rain, IDW, comparison



Spatial trend surface

- Assume some function of X and Y coordinates fits the data
- often a low order polynomial (linear or quadratic)

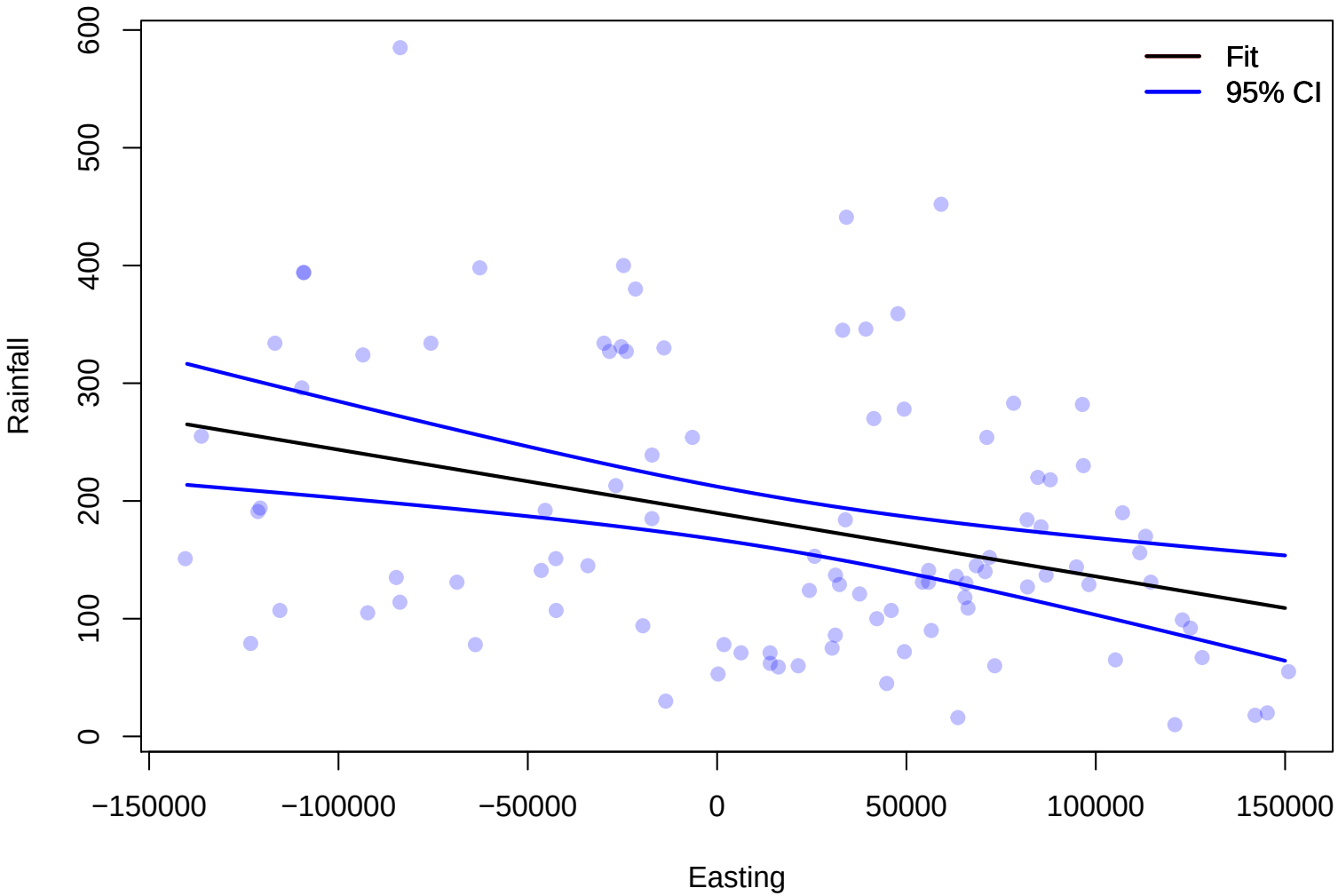
$$\begin{aligned} Z(\boldsymbol{s}_i) &= \beta_0 + \beta_1 X_i + \beta_2 Y_i + \varepsilon_i, \text{ or} \\ Z(\boldsymbol{s}_i) &= \beta_0 + \beta_1 X_i + \beta_2 Y_i + \beta_3 X_i^2 + \beta_4 Y_i^2 + \beta_5 X_i Y_i + \varepsilon_i, \end{aligned}$$

- only used for predicting $\hat{Z}(\boldsymbol{s}_i)$
- not doing any test or inference, so don't worry about correlation in ε's
- accounting for correlation, i.e. using GLS, will give better estimates of $\hat{\beta}$'s.
- Potential advantages over inverse distance weighting:
  - Can estimate Var ε
  - Can construct prediction intervals for $\hat{Z}(\boldsymbol{s}_i)$:
  - $\hat{Z}(\boldsymbol{s}_i) \pm T_{1-\alpha/2} \sqrt{s^2 + \text{Var } \hat{Z}(\boldsymbol{s}_i)}$

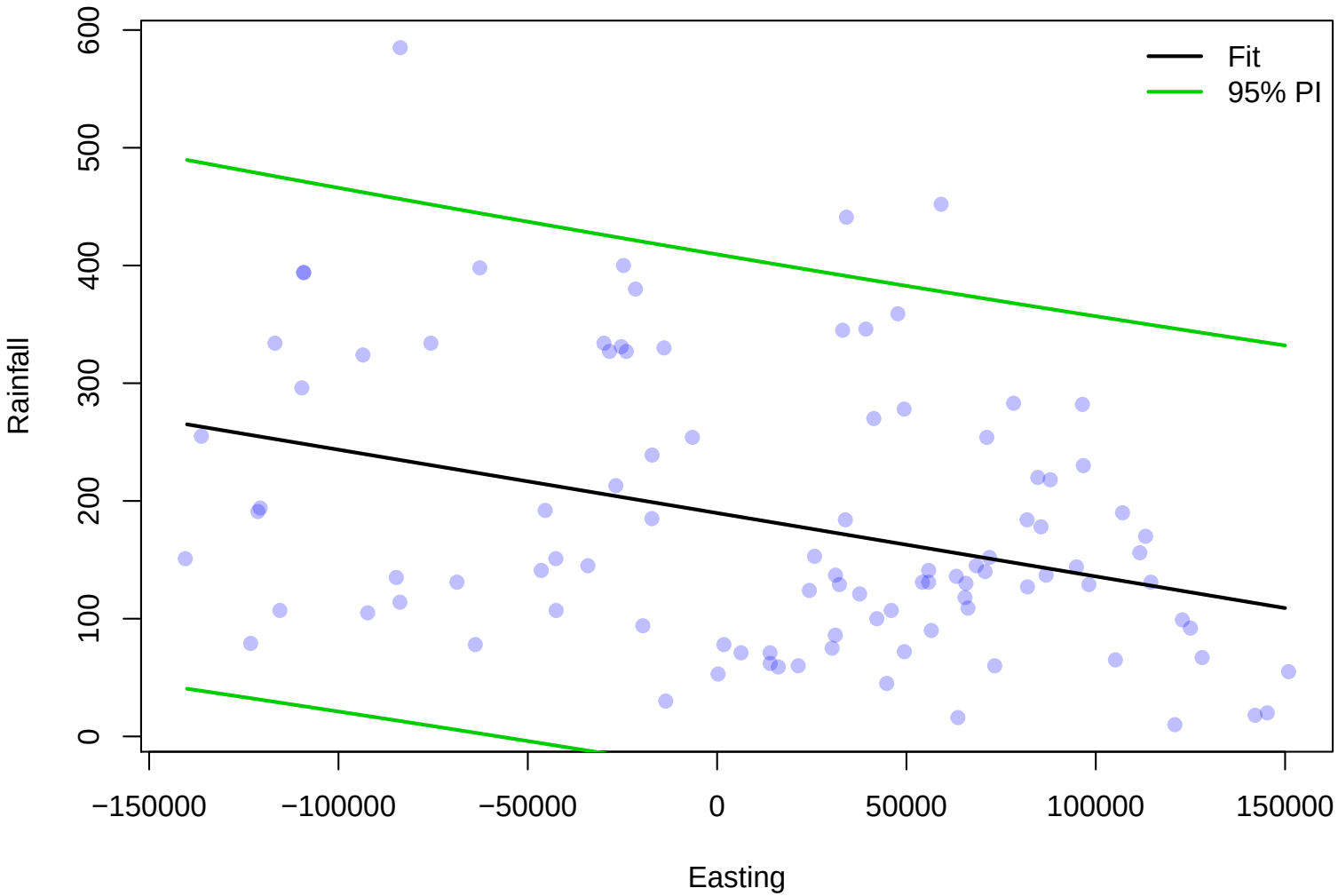
Spatial trend surface

- Confidence and Prediction intervals
- Reminder: can interpret a fitted regression line two ways
  - Predict average Y at some new X
    - Uncertainty only in regr. coefficients ("the line")
    - If I collected a second set of n obs, how similar is $\hat{Y}$?
    - Decreases as n increases
    - se of a mean, confidence interval for $\hat{Y}$
  - Predict a new observation at some new X
    - Uncertainty in both the line and obs around the line
    - Before sampling a new obs, how accurate is prediction?
    - Usually, very similar to s (rMSE), never smaller
    - sd of a predicted observation, prediction interval for $\hat{Y}$

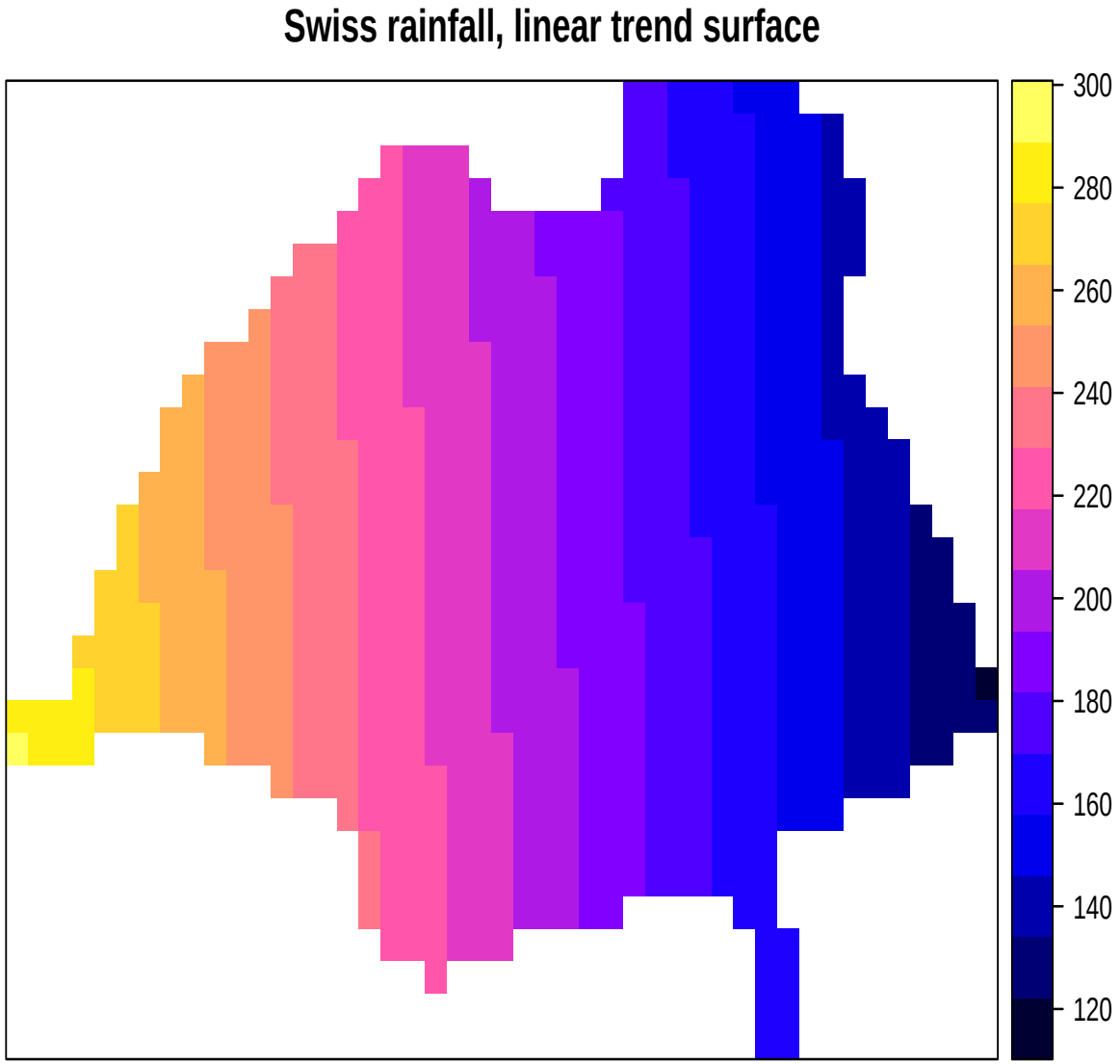
Confidence interval: Swiss rain



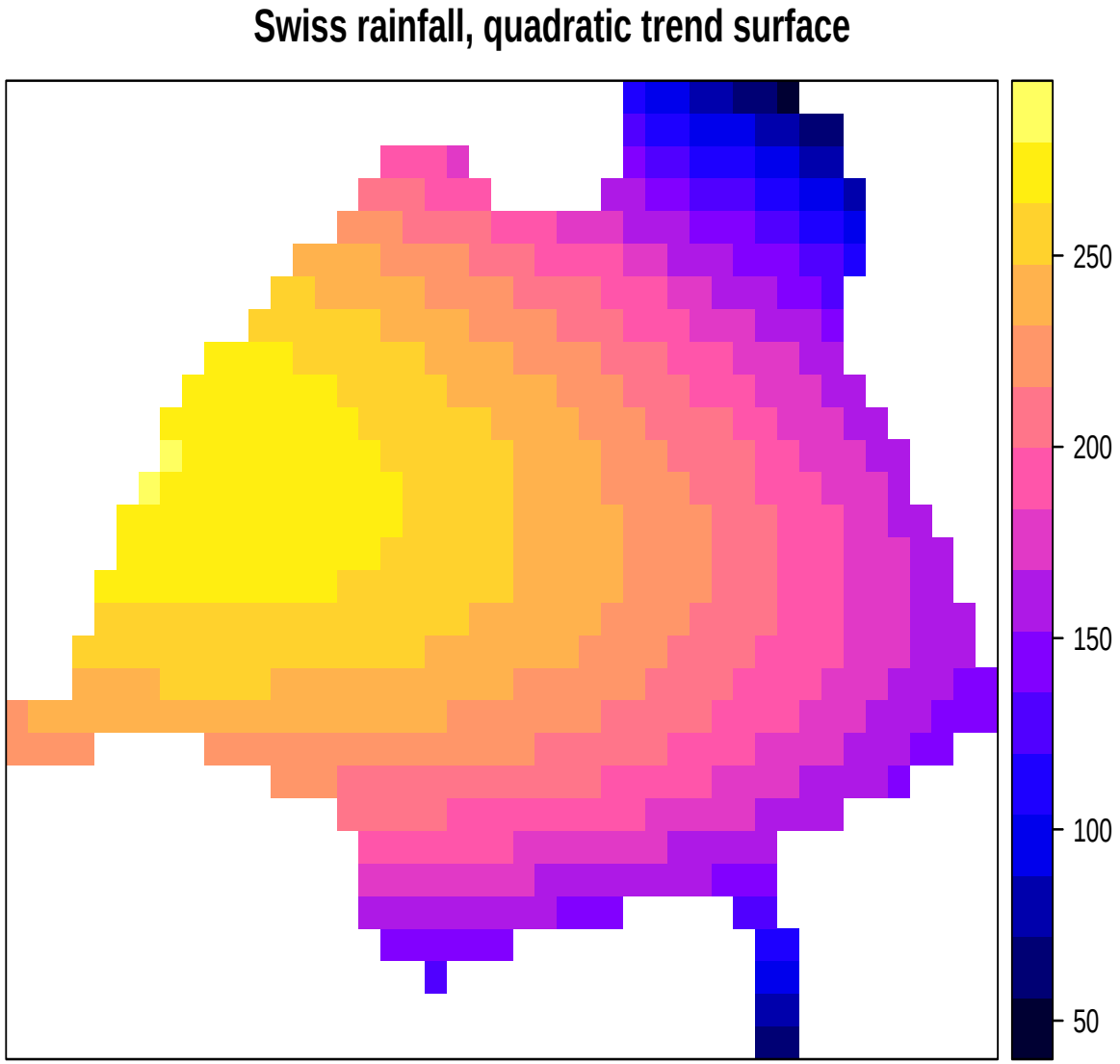
Prediction interval: Swiss rain



Swiss rain, linear TS

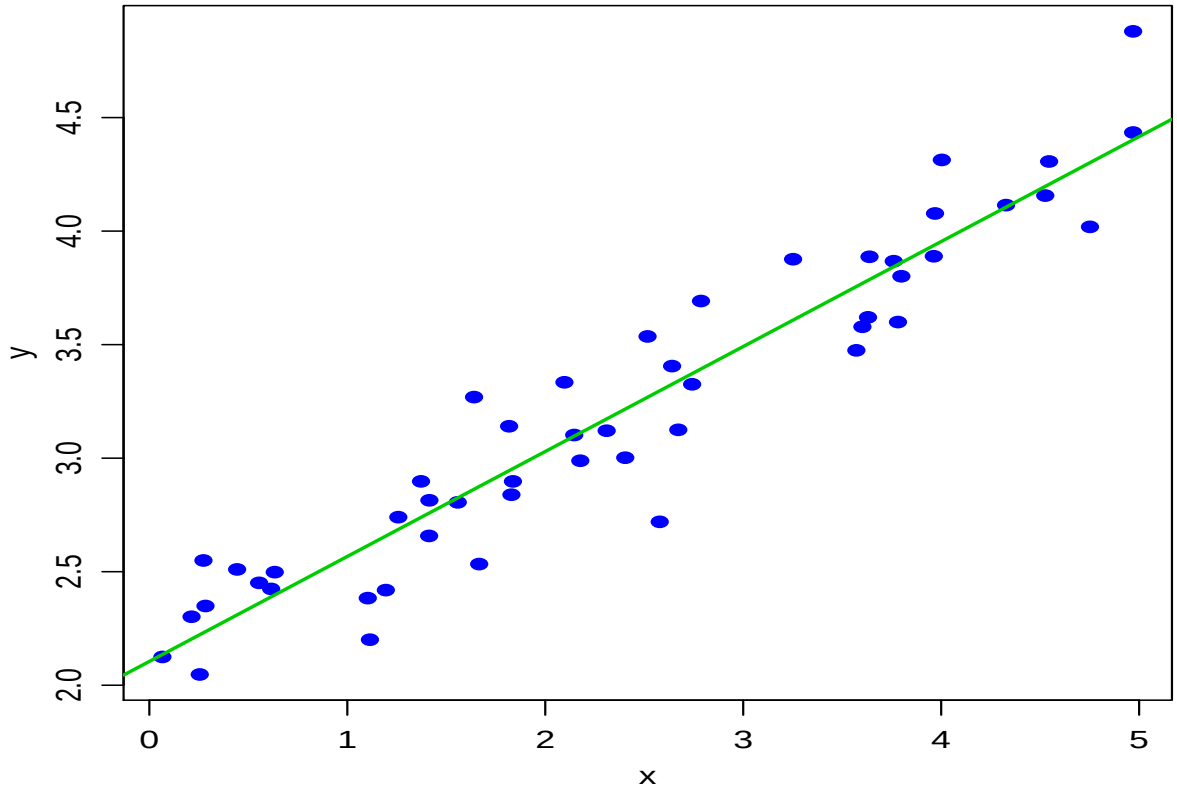


Swiss rain, quadratic TS



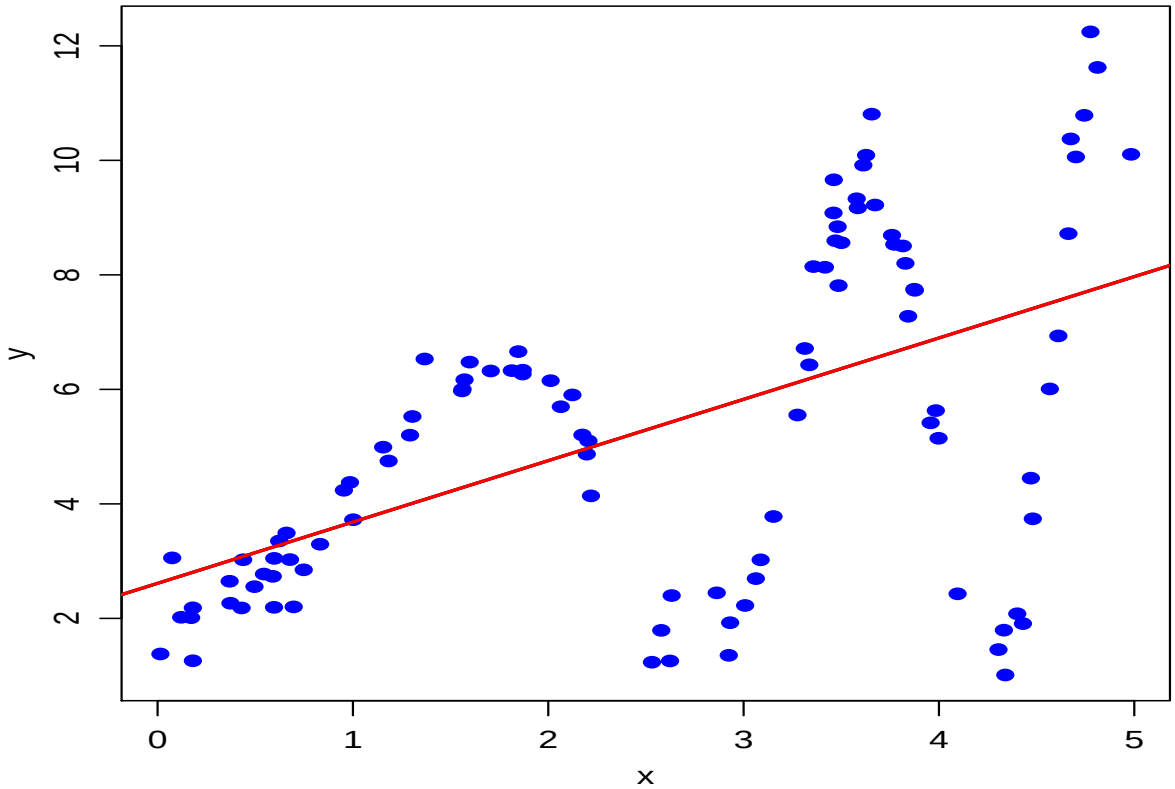
Splines: more flexible regression functions

- Concepts only. Details require a lot of intricate math and stat theory
- Consider response Y and one predictor X
- Sometimes a simple model is great



Splines: more flexible regression functions

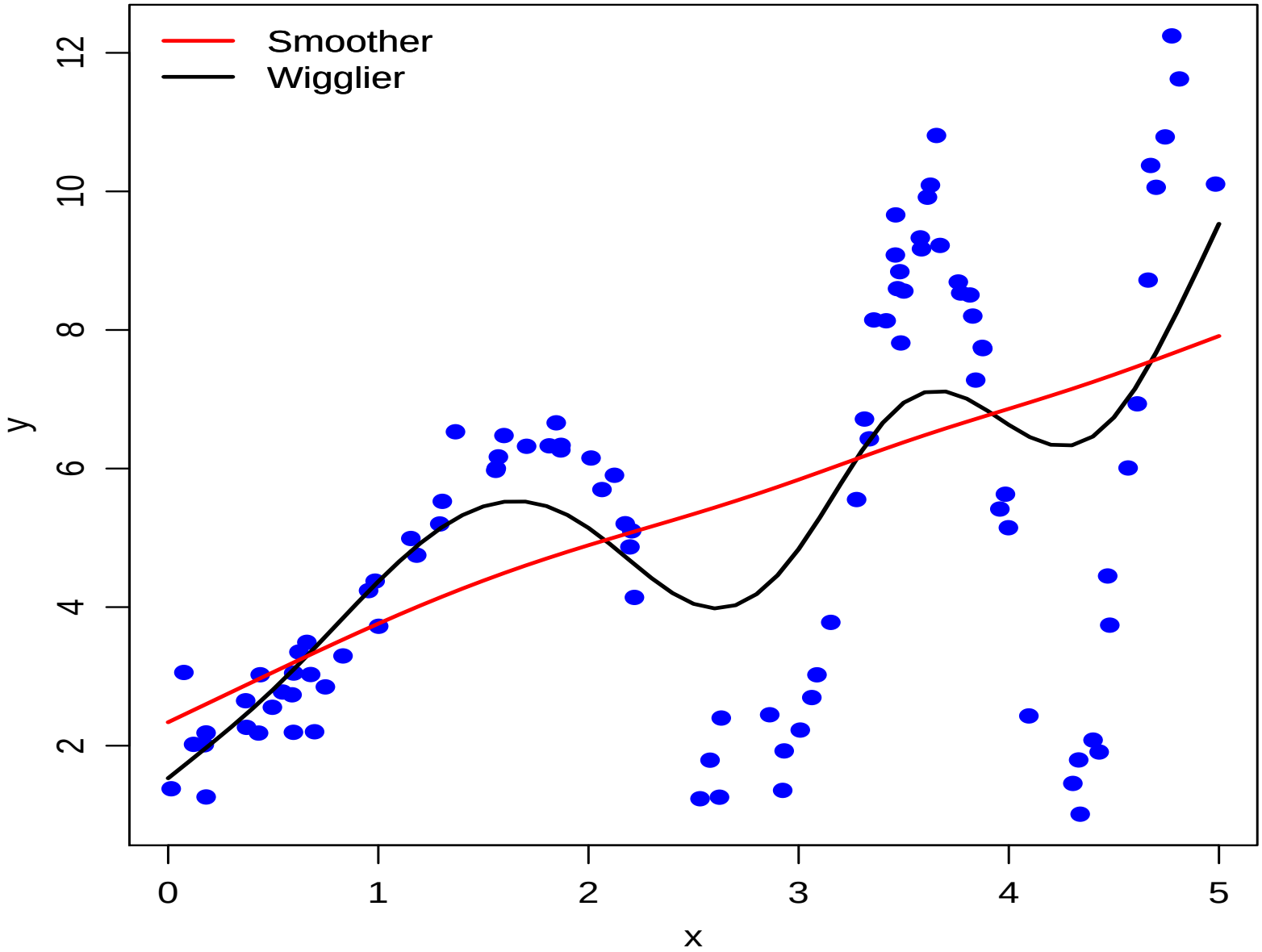
- And sometimes not



Splines: more flexible regression functions

- How to model relationship between Y and X, especially to predict?
  - If subject-matter-based model, use it!
  - Fit a higher order polynomial (quadratic, cubic)
  - Non-parametric regression: smooth the data
- Various NP regression methods. Focus on smoothing splines
- Concept: put together many models for small pieces of the data
- Need to choose number of small pieces
  - fewer pieces: smoother curve, closer to linear
  - more pieces: wigglier curve, closer to data

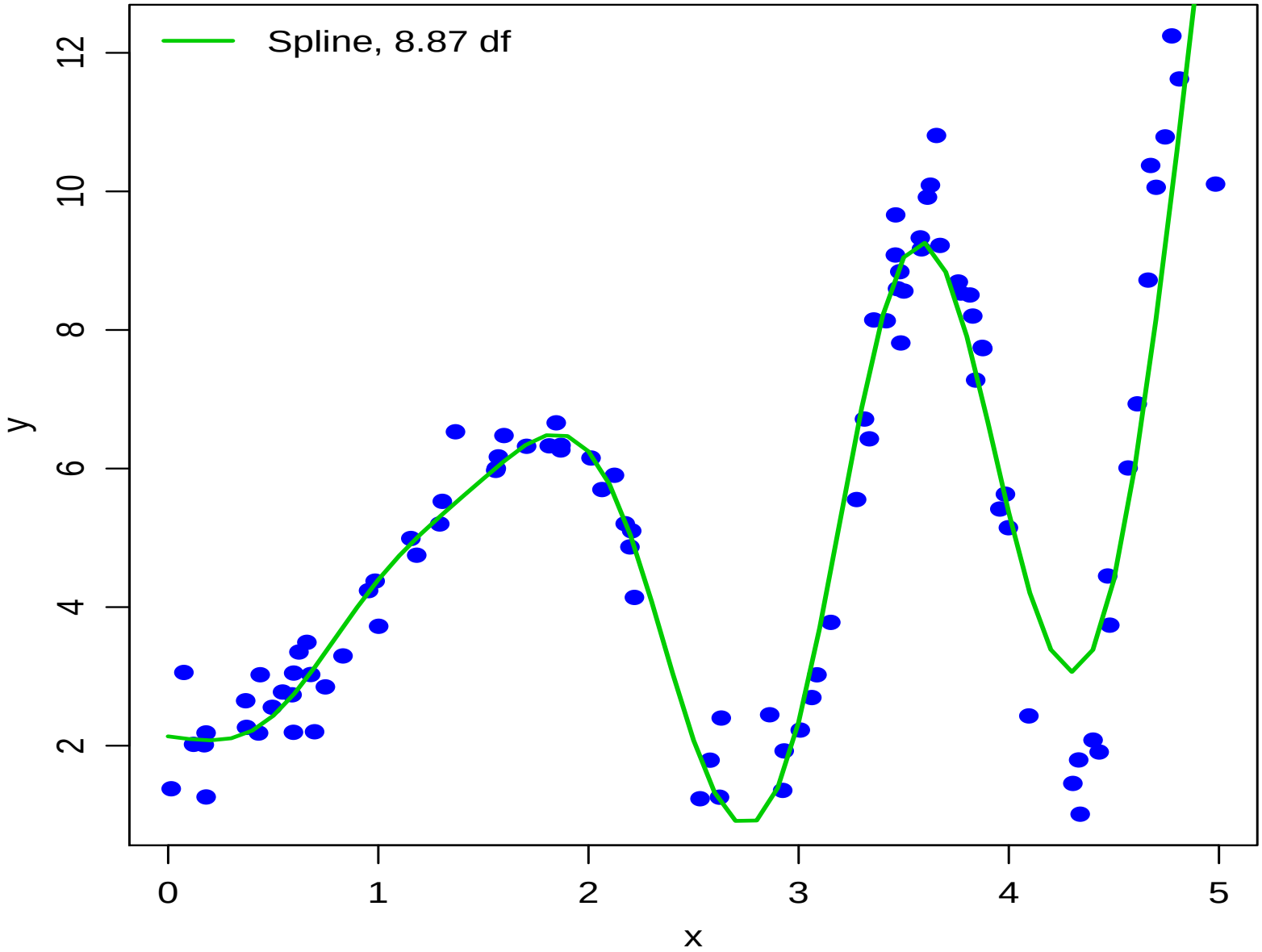
Spline fits



Spline fits

- How to choose how smooth/wiggly?
- not easy
- Too smooth is obviously bad
- Extemely wiggly effectively connects the dots
  - also bad - predictions of new obs. are inaccurate
  - overfitting the observed data
  - treating "noise" as signal.
- One common solution: cross validation
  - leave out an obs, fit a model, predict left obs.
  - put back, leave out next obs, $\cdots$
  - right choice is the value that makes good preds. of all the left-out obs
- splines require more data than when you know the model

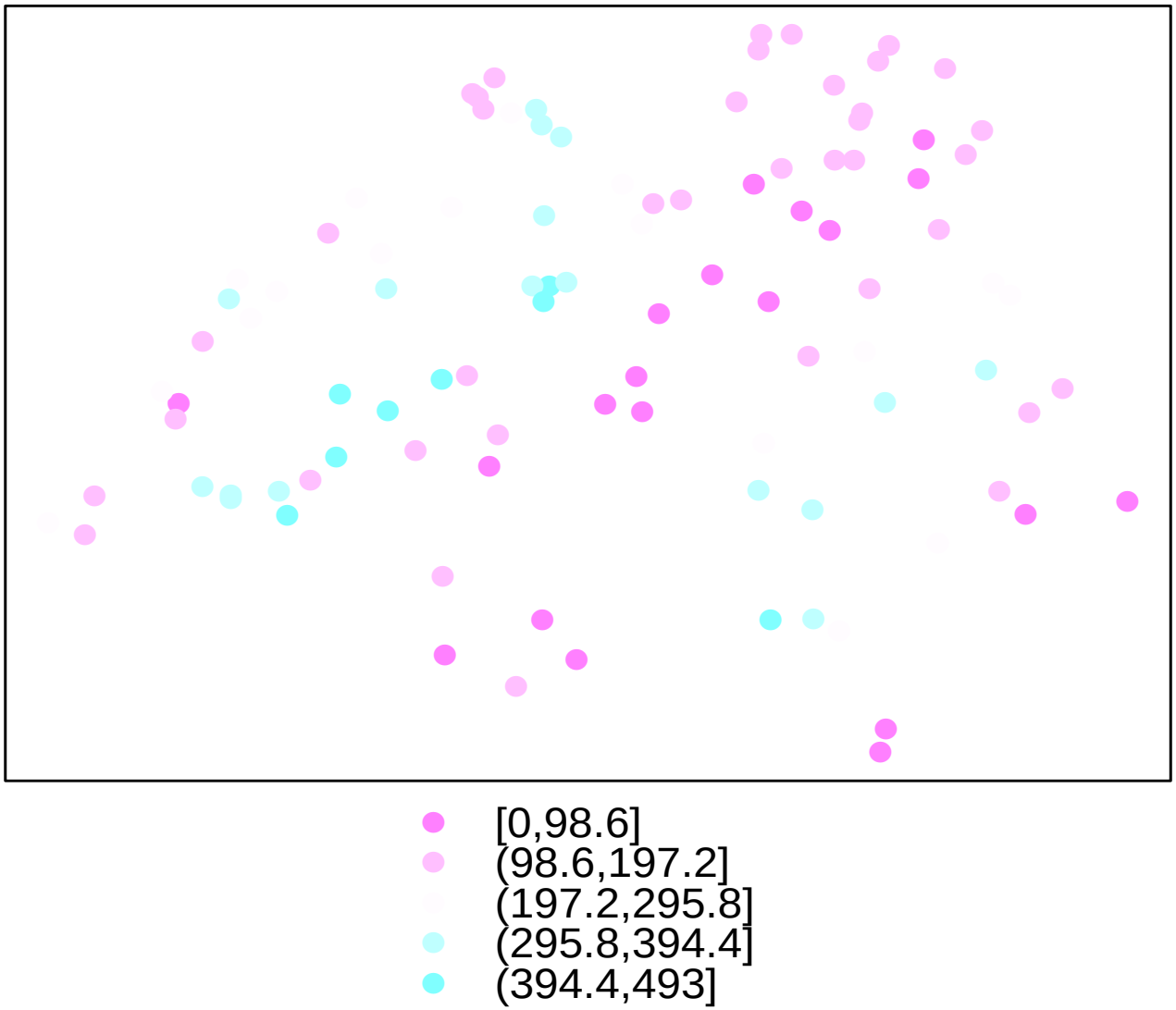
Spline fits



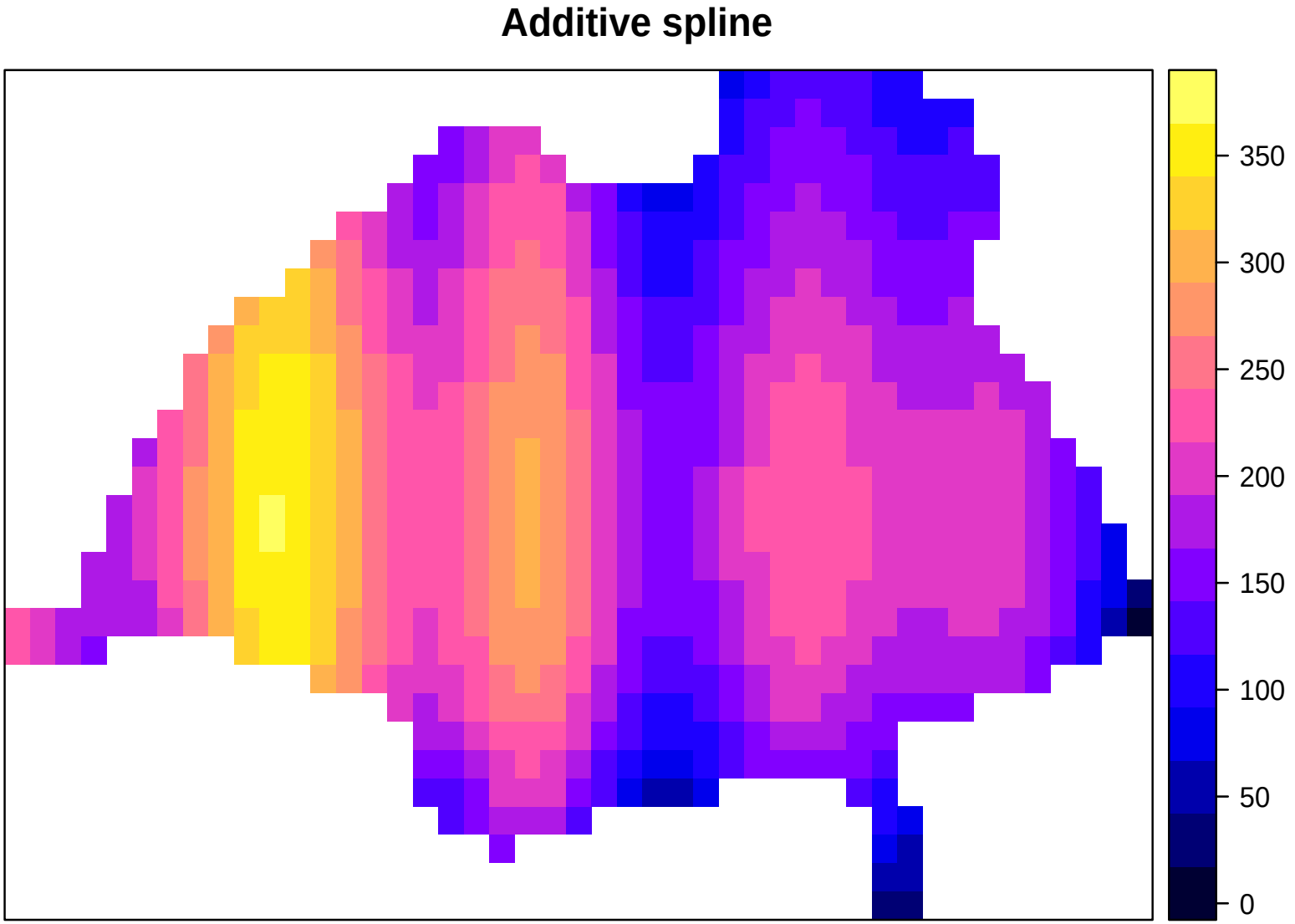
Spline fits

- Two ways to extend to spatial data
- Additive splines
  - spline fn of X coordinate: describes pattern in X
  - spline fn of Y coordinate: describes pattern in Y
  - Add them together
- depends on axis directions. Assumes pattern along the axes

Swiss rainfall data



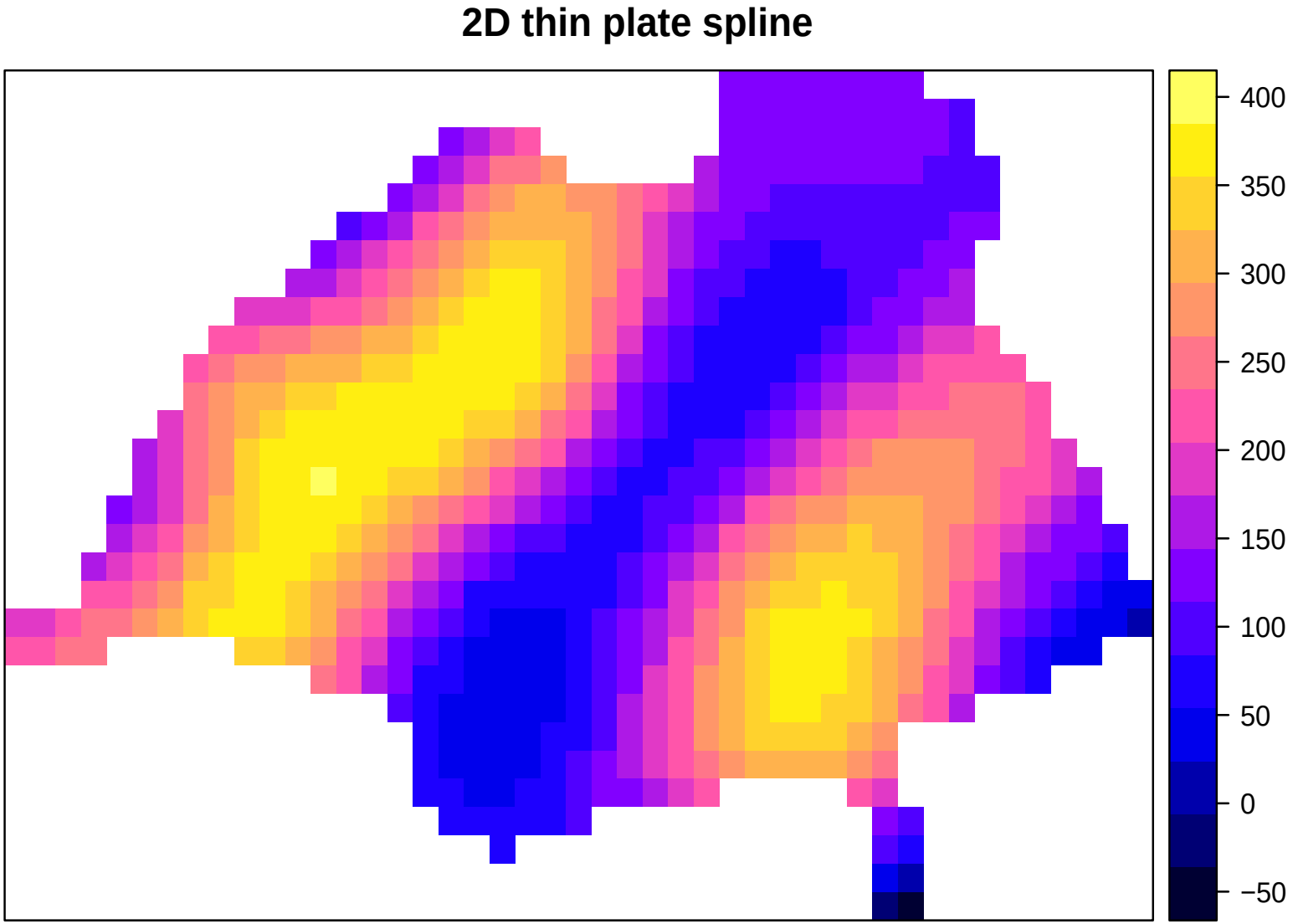
Swiss rain, Spline fit: s(x) + s(y)



Spline fits

- Two ways to extend to spatial data
- thin plate spline
  - think of a sheet of paper or thin sheet of metal
  - drape over the data, allow to wiggle
  - models pattern in all directions simultaneously
  - not dependent on axis directions
  - requires much more data than additive splines

Swiss rain, Spline fit: s(x,y)



Models for data

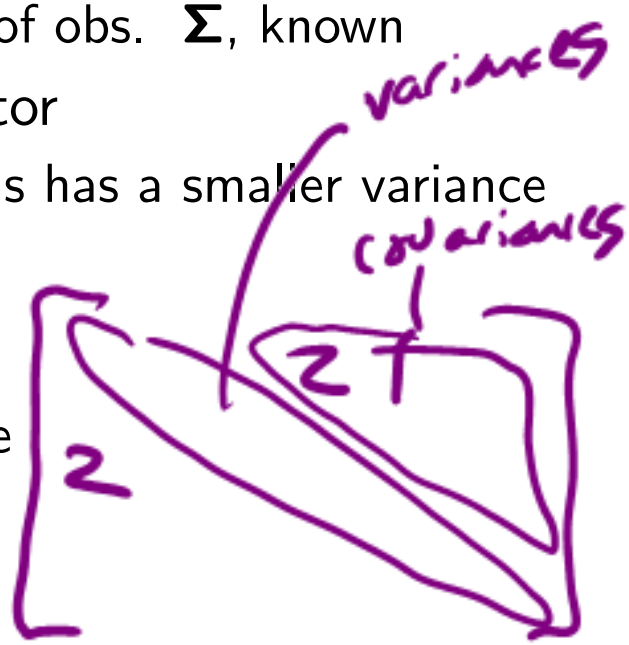
- IDW: no model
- trend surface: $\boldsymbol{Z(s)} = \beta_0 + f(\boldsymbol{s}) + \varepsilon$
  - all the spatial "action" is in $f(\boldsymbol{s})$
  - Have to choose form of $f(\boldsymbol{s})$
    - $\beta_1 X + \beta_2 Y$
    - $\beta_1 X + \beta_2 Y + \beta_3 X^2 + \beta_4 Y^2 + \beta_5 XY$
    - $s(X) + s(Y)$
    - $s(X, Y)$
  - given form of model, can easily estimate unknown parameters, e.g., β_1, β_2, or the parameters in $s()$.
- kriging: simple, ordinary $\boldsymbol{Z(s)} = \beta_0 + \varepsilon$
  - ε are correlated. nearby observations more so.
  - all the spatial "action" is in the correlations
- universal kriging: $\boldsymbol{Z(s)} = \beta_0 + f(\boldsymbol{s}) + \varepsilon$, ε correlated

Kriging

- Original motivation:
  - underground gold mining. gold content varies along a rock face
  - want to predict where highest gold content
  - and / or average gold content in an area
  - sample a small fraction of the rock face
  - prediction problem: predict $\boldsymbol{\hat{Z}(s)}$ at new locations given data
- Danie Krige: treat $\boldsymbol{Z(s)}$ as spatially correlated collection of r.v.'s
- derive optimal predictor
- original paper: 1951, So. African mining journal
- procedure now known as kriging

Kriging

- Simplest setup of the problem:
  $\boldsymbol{Z(s)} = \beta_0 + \varepsilon$, $\varepsilon \sim N(\underline{0}, \boldsymbol{\Sigma})$, β_0, $\boldsymbol{\Sigma}$ known
- In words:
  - observations are spatially correlated r.v.'s
  - mean β_0 known
  - covariances (or correlations) between all pairs of obs. $\boldsymbol{\Sigma}$, known
- Can derive: Kriging is the optimal linear predictor
  - No other linear combination of the observations has a smaller variance
- predictions are weighted average of the obs.
- weights are functions of the spatial pattern
  - When little spatial pattern, $\rightarrow$ regional average
  - When strong spatial pattern, $\rightarrow$ local average
- weights can be > 1 or < 0
  - predictions can exceed range of observations



$Cov(Z_1, Z_2) = \sqrt{Var Z_1 \cdot Var Z_2}\, Corr(Z_1, Z_2)$

Kriging notation

- Use vectors and matrices to describe the data $\boldsymbol{Z(s)}$, their means $\boldsymbol{\mu}$, and their variance-covariance matrix, $\boldsymbol{\Sigma}$.
- $\boldsymbol{Z(s)} = \begin{bmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_n \end{bmatrix}$, $\boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{bmatrix}$, $\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{12} & \sigma_2^2 & \cdots & \sigma_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ \sigma_{1n} & \sigma_{2n} & \cdots & \sigma_n^2 \end{bmatrix}$
- $P(\boldsymbol{s}_0)$ is a function that predicts $Z(\boldsymbol{s}_0)$

$\sigma_{1A} = \sigma_1^2$

Kriging as making a good prediction

- What should we choose for $P(\boldsymbol{s}_0)$?
- Want a "good" prediction. Need to measure how good or how bad.
- In general, define a loss function, $L()$, that tells us how to measure good/bad.
- Kriging: use squared error loss

$$L\left(Z(\boldsymbol{s}_0), P(\boldsymbol{s}_0)\right) = \left(Z(\boldsymbol{s}_0) - P(\boldsymbol{s}_0)\right)^2$$

- $P(\boldsymbol{s}_0)$ depends on the data, so $L()$ is a random variable
- so define a good predictor as one that minimizes E $L()$
- That predictor is E $Z(\boldsymbol{s}_0) \mid \boldsymbol{Z(s)}$ "given"

Expected Z at new location given specific values of Z(s) at obs. locs.

Simple Kriging

- Kriging model: $\boldsymbol{Z(s)} = \mu(s) + \varepsilon(s)$
  where $\varepsilon(s)$ are correlated (spatial pattern)
- $\mu(s)$ is known, initially assume $\boldsymbol{\Sigma}$ is known
- can derive:

$$P(\boldsymbol{s}_0) = \mu(\boldsymbol{s}_0) + \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1} (\boldsymbol{Z(s)} - \mu(s))$$

,

  - Derivation done in S&G, p. 223
  - $\boldsymbol{\sigma}$ is vector of covariances: Cov $(Z(\boldsymbol{s}_0), \boldsymbol{Z(s)})$
  - $\boldsymbol{\Sigma}$ is the Var-Cov matrix of the observations
- Least Squares regression: same loss function
  - Used to writing $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$
  - Algebra: same as $\hat{Y}_i = \bar{Y} + \sigma_{xy}(\sigma_X^2)^{-1}(X_i - \bar{X})$

Simple Kriging

- This is the best predictor if $\boldsymbol{Z(s)}$ is Gaussian = multivariate normal
- best linear predictor if $\boldsymbol{Z(s)}$ is not Gaussian
- Can also estimate prediction variance

$$\sigma^2(\boldsymbol{s}_0) = \sigma^2 - \boldsymbol{\sigma}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\sigma}$$

prediction var = $\sigma^2 + \text{Var}\,\hat{Y}$

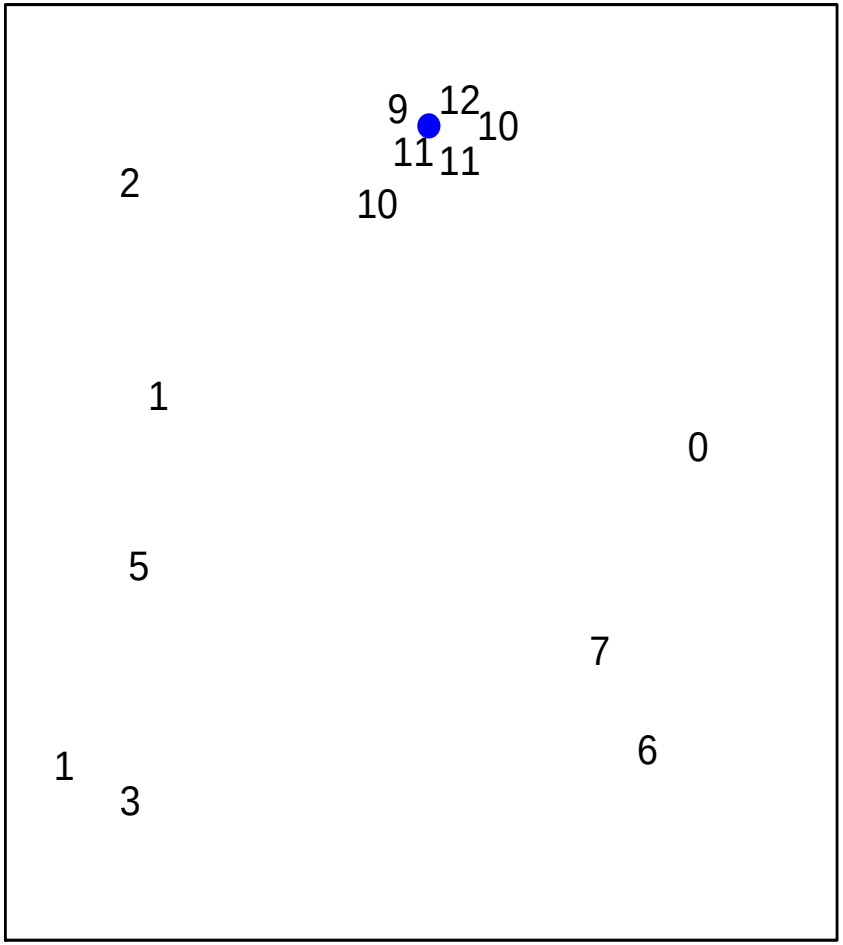
quadratic form ≥ 0

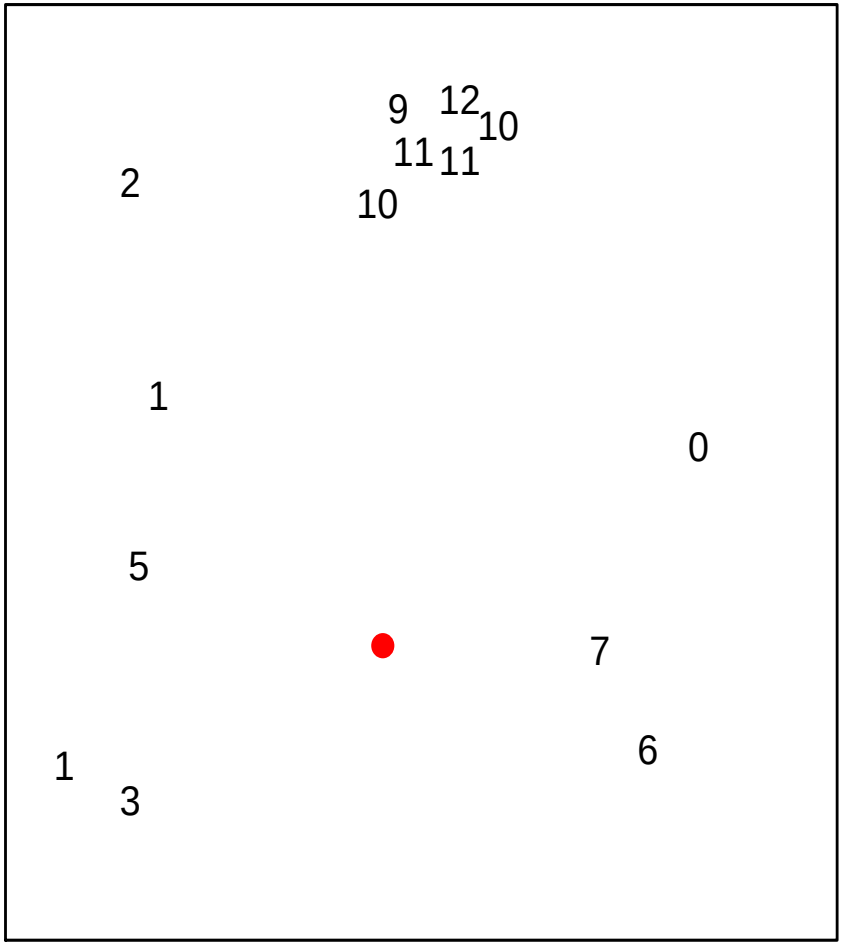
  - This is the variance in the prediction conditional on (i.e., given) observed values
- Looks a bit unusual: usually add variances
- $\boldsymbol{\sigma}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\sigma}$ large when prediction loc. is highly corr. with nearby locs
- Reduces uncertainty in the prediction

10 x 12 8

Simple Kriging

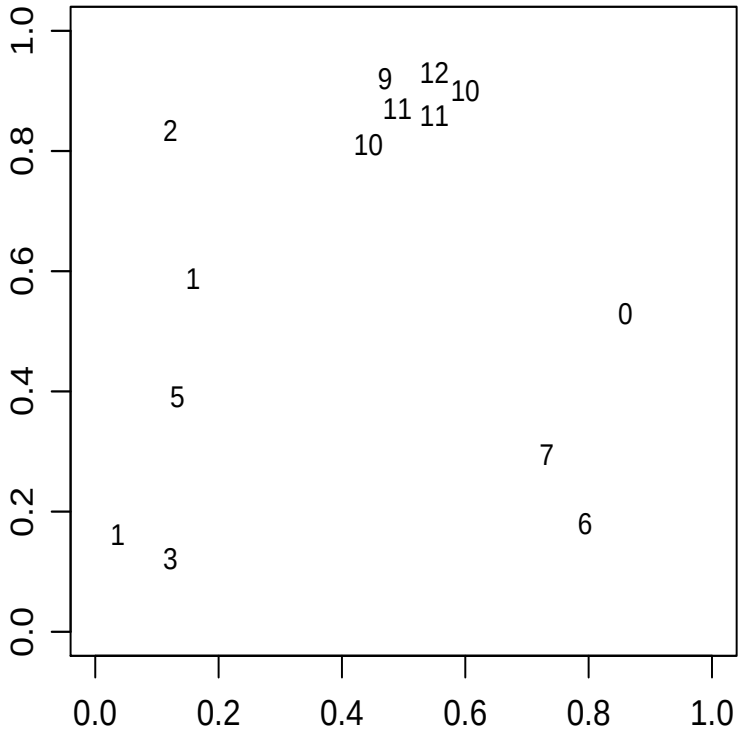
$$P(s_0) = w_1 Z(s_1) + w_2 Z(s_2) \cdots$$





Simple Kriging: example

- Understanding the prediction in a simple situation
  - Our population: constant mean.
  - Our data: not same value because of random variation



Simple Kriging: example

- The prediction is:

$$P(\boldsymbol{s}_0) = \mu + \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1} (\boldsymbol{Z}(\boldsymbol{s}) - \boldsymbol{\mu})$$

- This is a weighted average of the deviations from the mean, $\boldsymbol{\mu}$

$$P(\boldsymbol{s}_0) = \mu + \boldsymbol{w} (\boldsymbol{Z}(\boldsymbol{s}) - \boldsymbol{\mu})$$

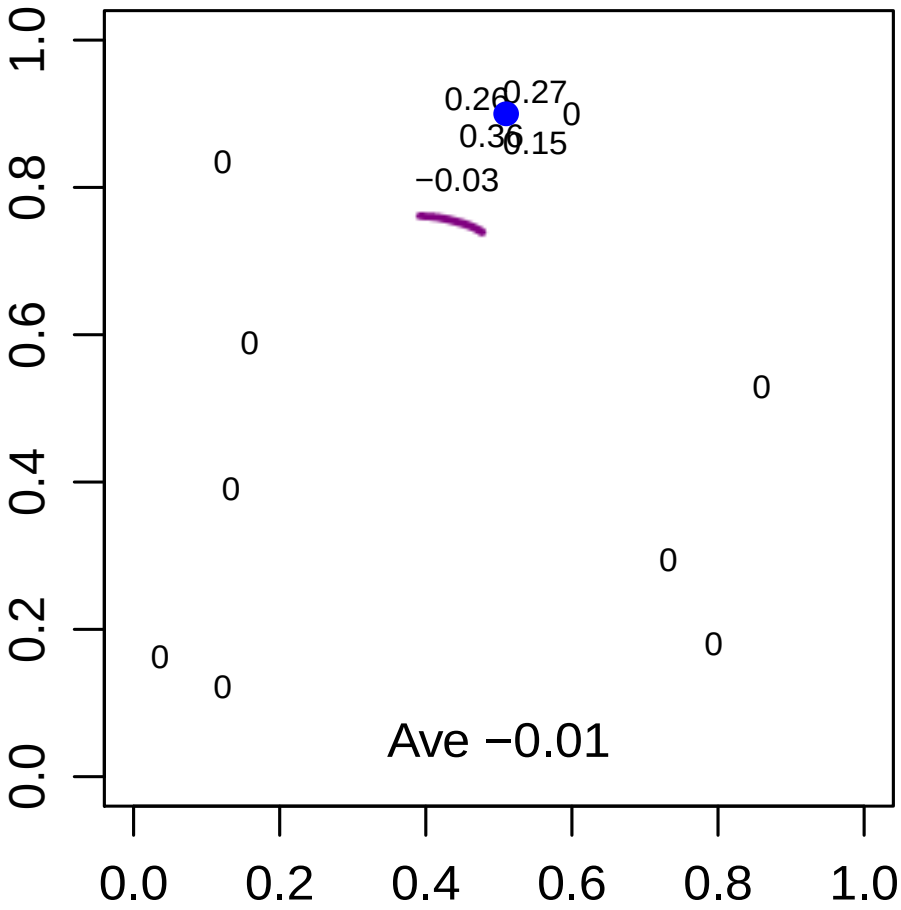
  where the weights, $\boldsymbol{w}$, depend on the correlations: $\boldsymbol{w} = \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1}$

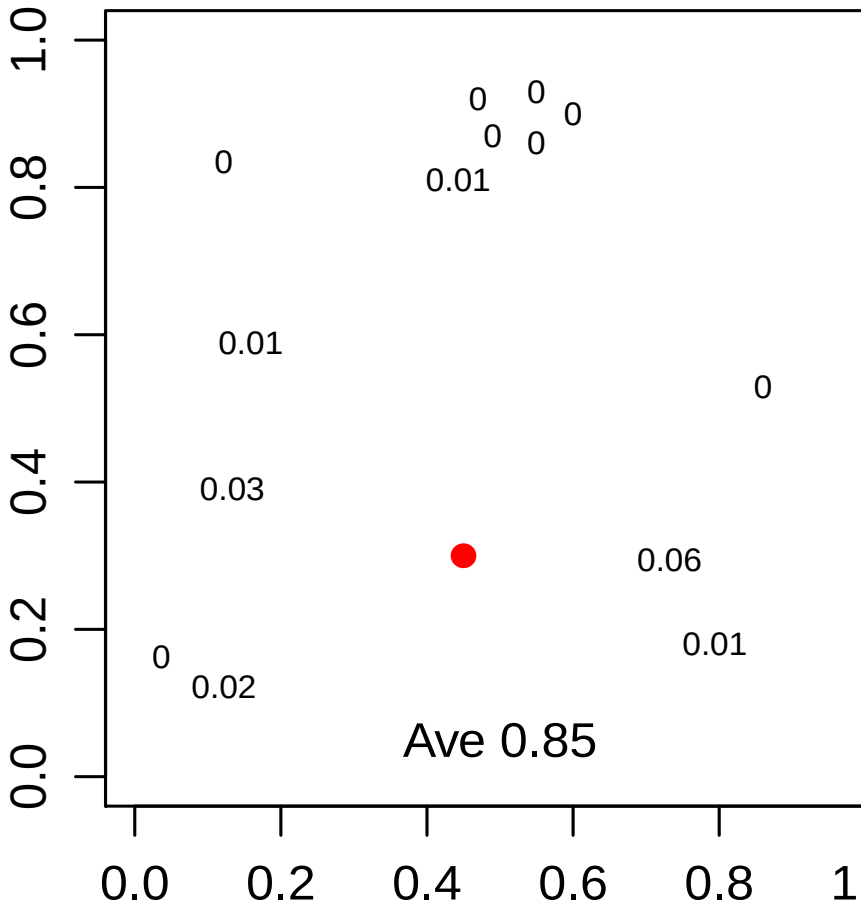
- Can rewrite as a weighted average of n $Z(s)$ values and the mean, μ

$$P(\boldsymbol{s}_0) = \boldsymbol{w}\boldsymbol{Z}(\boldsymbol{s}) + (1 - \Sigma \boldsymbol{w})\boldsymbol{\mu}$$

- look at those weights for predictions at two observations:
  - blue location: close to measured locations
  - red location: distant from all measured locations

Simple Kriging: example





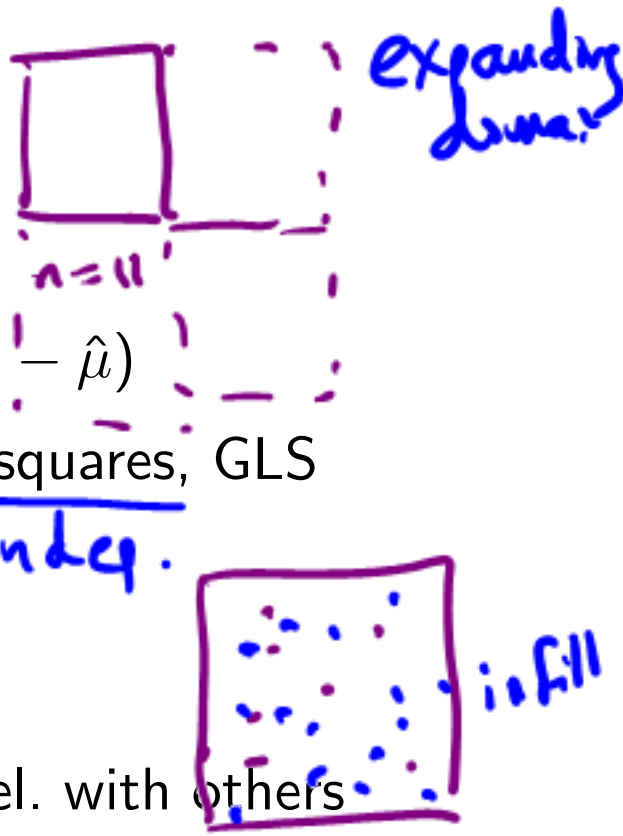
Ordinary Kriging

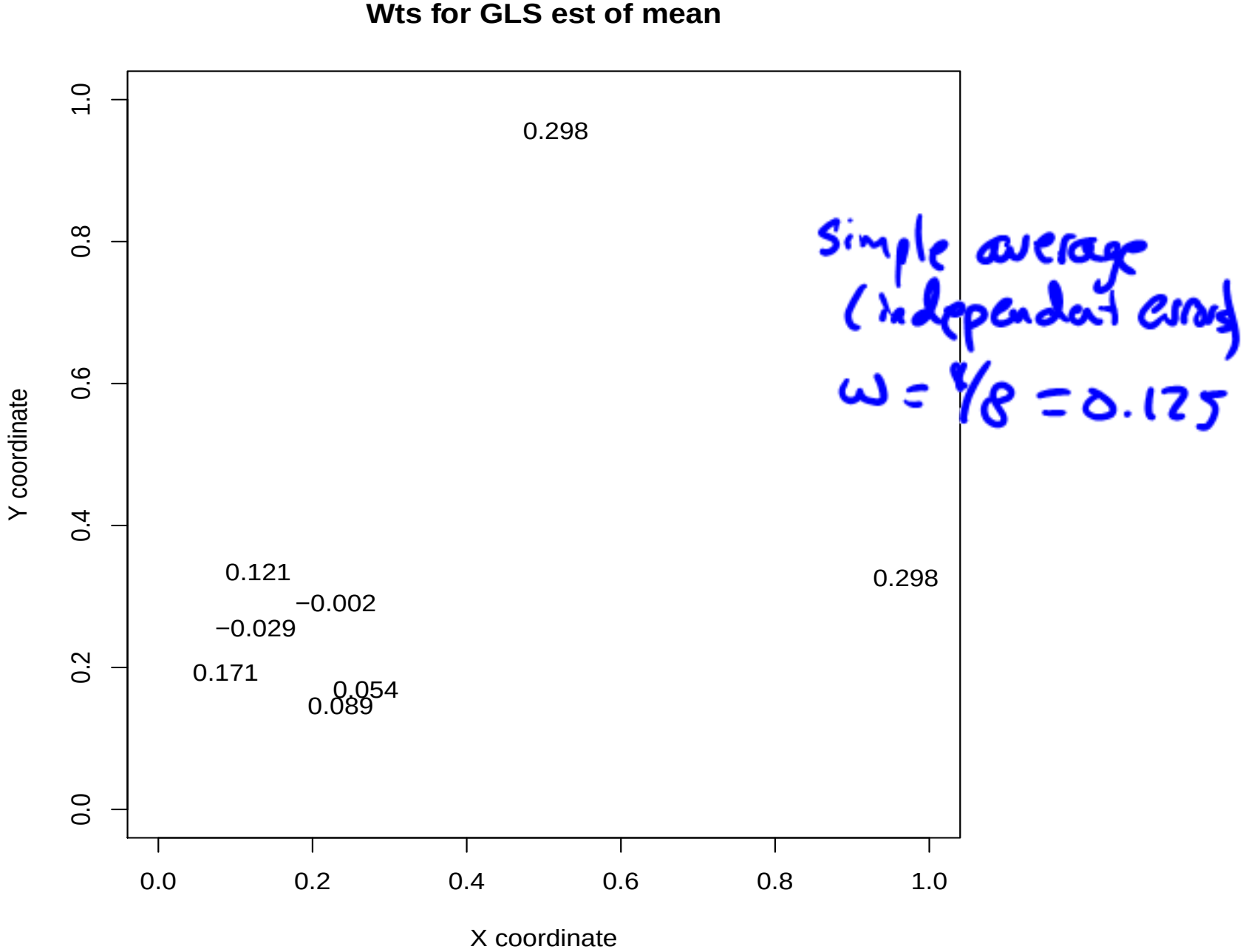
- The problem with simple kriging is that $\mu(\boldsymbol{s}_0)$ usually not known
- Ordinary Kriging: estimate $\hat{\mu}(\boldsymbol{s}_0)$
- slightly different statistical properties
  - no best linear predictor
  - but O.K. is best linear unbiased predictor

$$P(\boldsymbol{s}_0) = \hat{\mu}(\boldsymbol{s}_0) + \boldsymbol{\sigma}' \boldsymbol{\Sigma}^{-1} (\boldsymbol{Z}(\boldsymbol{s}) - \hat{\mu})$$

, where $\hat{\mu}(\boldsymbol{s}_0)$ is estimated by generalized least squares, GLS

  - For $\boldsymbol{Y} = \boldsymbol{X}\beta + \varepsilon$, OLS: $\hat{\beta} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}$
  - In general, GLS: $\hat{\beta} = (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{Y}$
  - To estimate $\hat{\mu}$, $\hat{\mu} = (\mathbf{1}'\boldsymbol{\Sigma}^{-1}\mathbf{1})^{-1}\mathbf{1}'\boldsymbol{\Sigma}^{-1}\boldsymbol{Z}(\boldsymbol{s})$
- Consequence of GLS is less weight on obs. correl. with others
- Picture on next slide




Wts for GLS est of mean
0.298
0.121
−0.002
−0.029
0.171
0.054
0.089
0.298
Y coordinate
X coordinate
0.0
0.2
0.4
0.6
0.8
1.0
Simple average
(Independent case)
w = 1/8 = 0.125

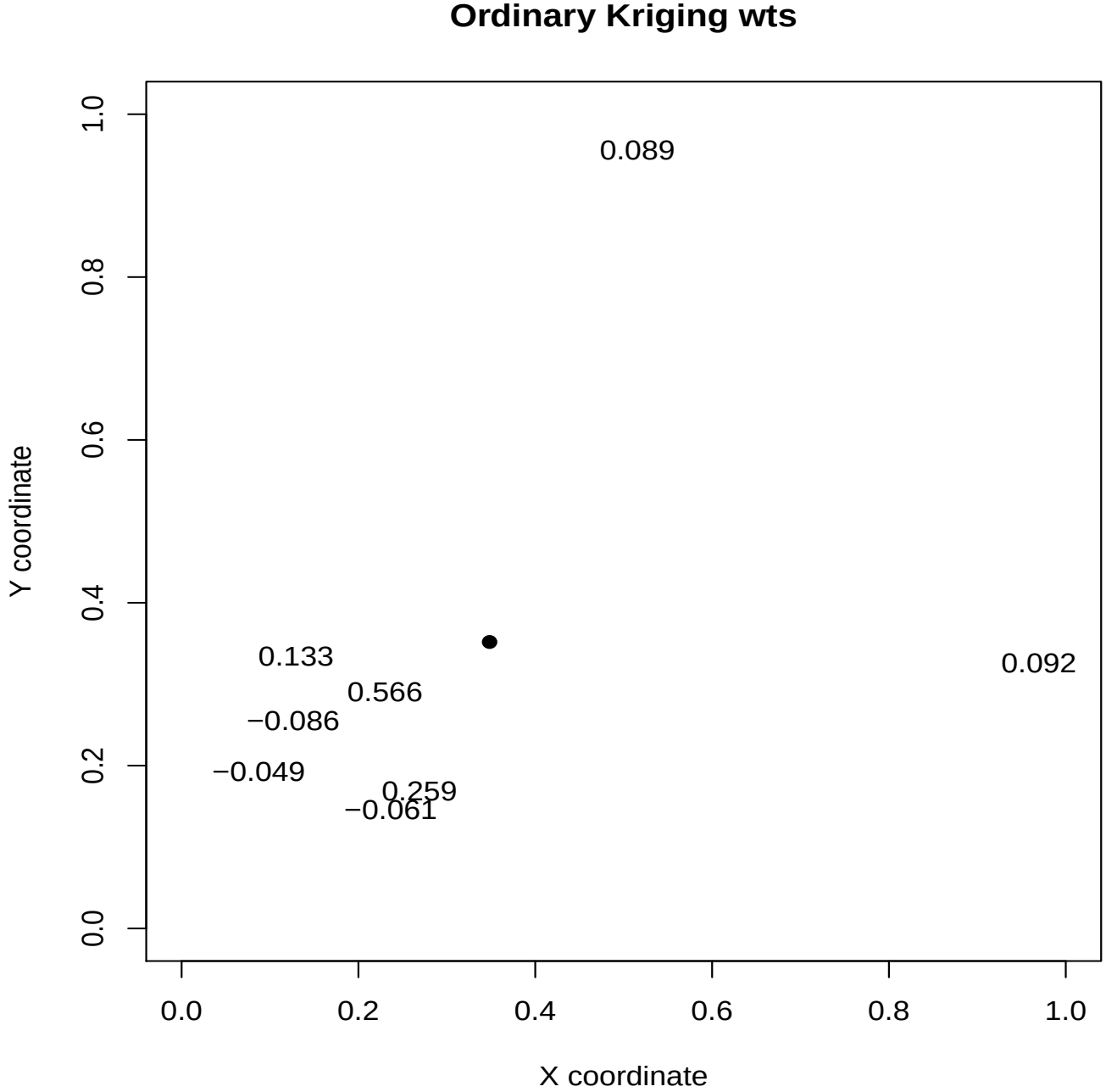
- Useful insight: $\boldsymbol{\sigma}'\boldsymbol{\Sigma}^{-1}$ is a row vector, so

$$P(\boldsymbol{s}_0) = \hat{\mu}(\boldsymbol{s}_0) + \boldsymbol{\lambda}'(\boldsymbol{Z}(\boldsymbol{s}) - \hat{\mu})$$

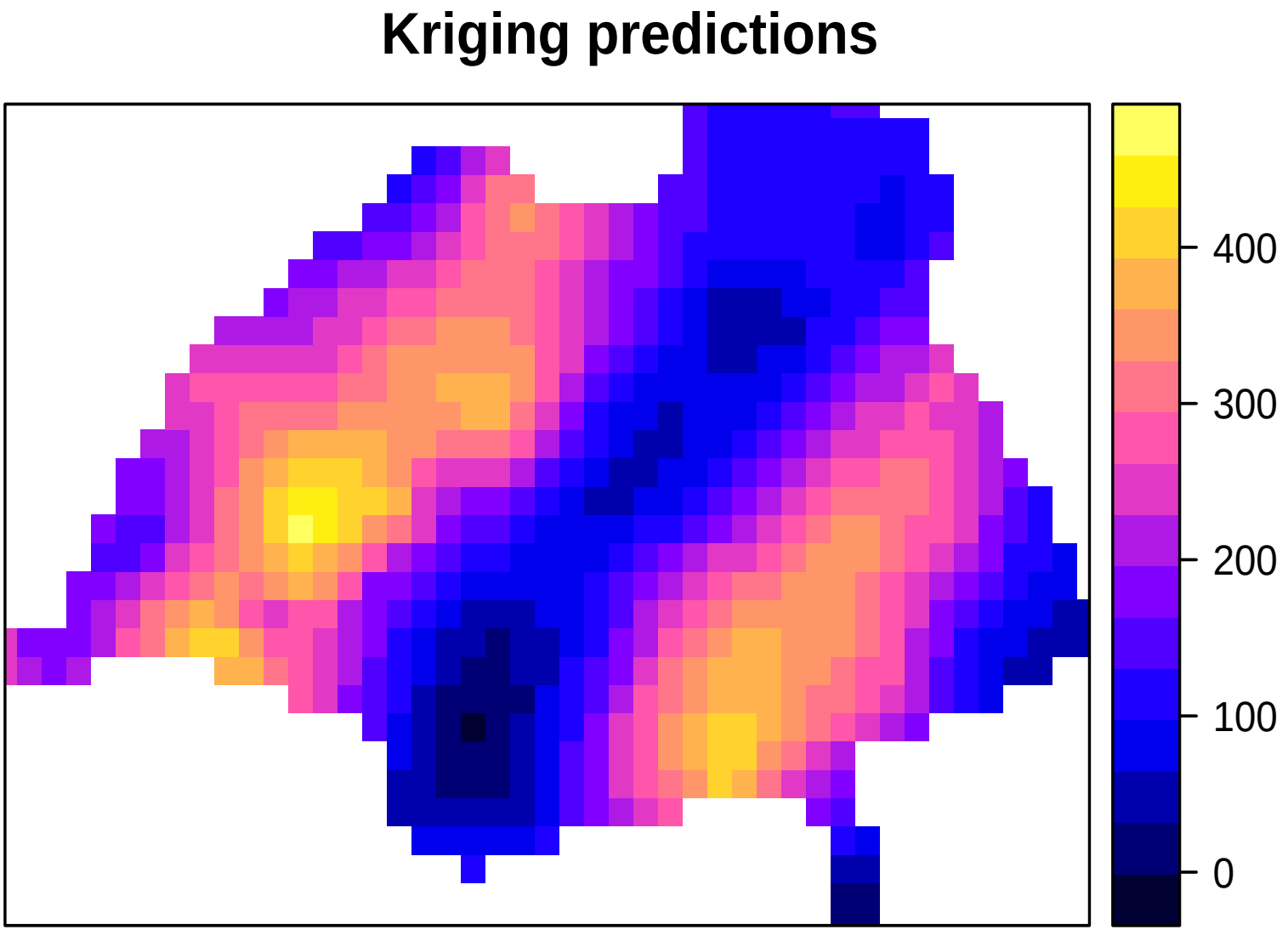
- values in $\boldsymbol{\lambda}$ depend on covariance btwn obs. values and covariance between prediction location and obs. values
- high for obs. close to prediction location
- values in $\boldsymbol{\lambda}$ may be negative, when obs. are "shadowed"
- Picture on next slide.
- Prediction variance:

$$\sigma^2(\boldsymbol{s}_0) = \sigma^2 - \boldsymbol{\sigma}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\sigma} + \frac{(1 - \mathbf{1}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\sigma})^2}{\mathbf{1}'\boldsymbol{\Sigma}^{-1}\mathbf{1}}$$

- S.K. prediction variance + addn. variance because est. μ.


Ordinary Kriging wts
0.089
0.133
0.566
−0.086
−0.049
0.259
−0.061
0.092
Y coordinate
X coordinate
0.0
0.2
0.4
0.6
0.8
1.0

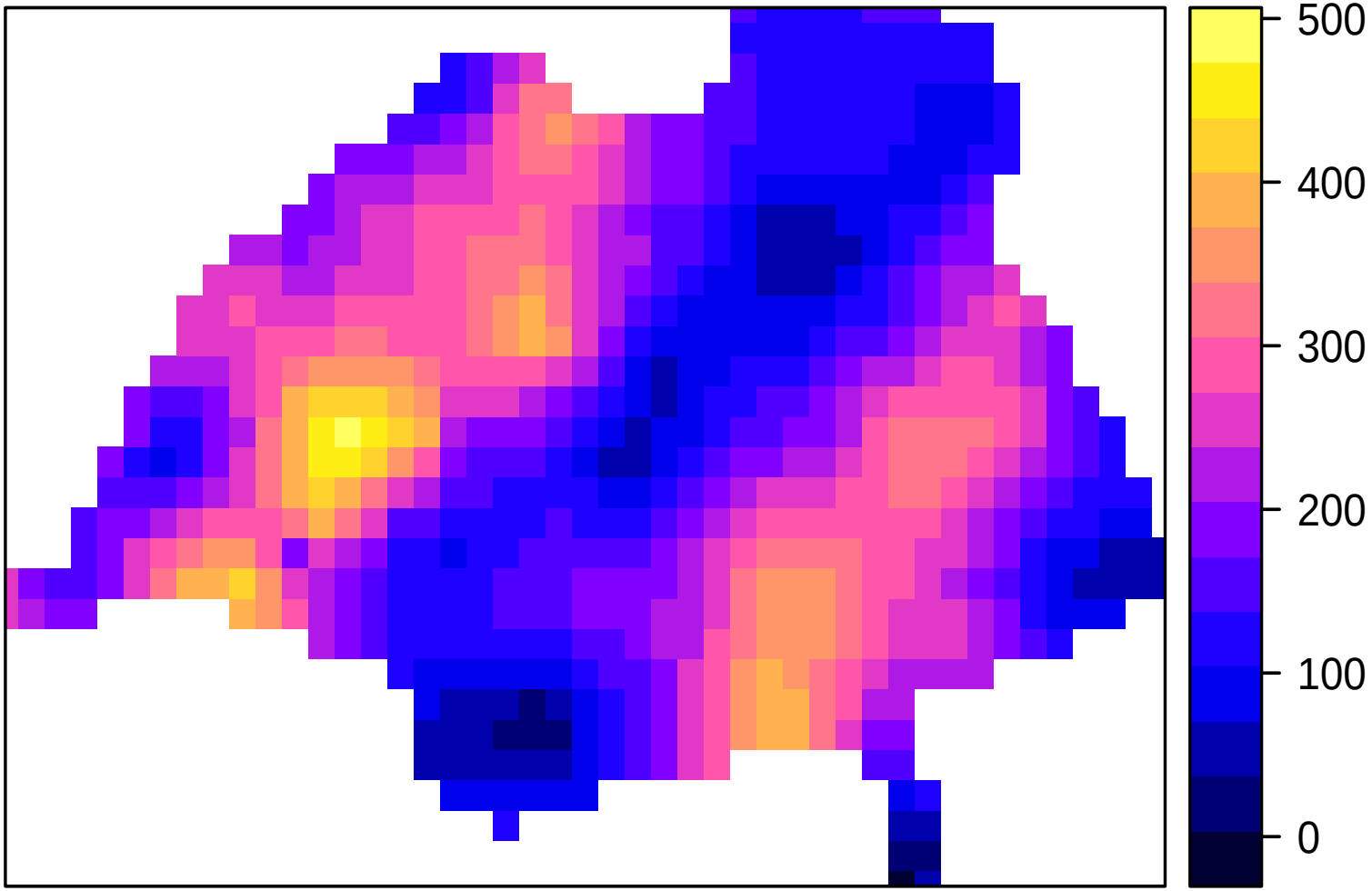
Swiss rainfall



Swiss rainfall

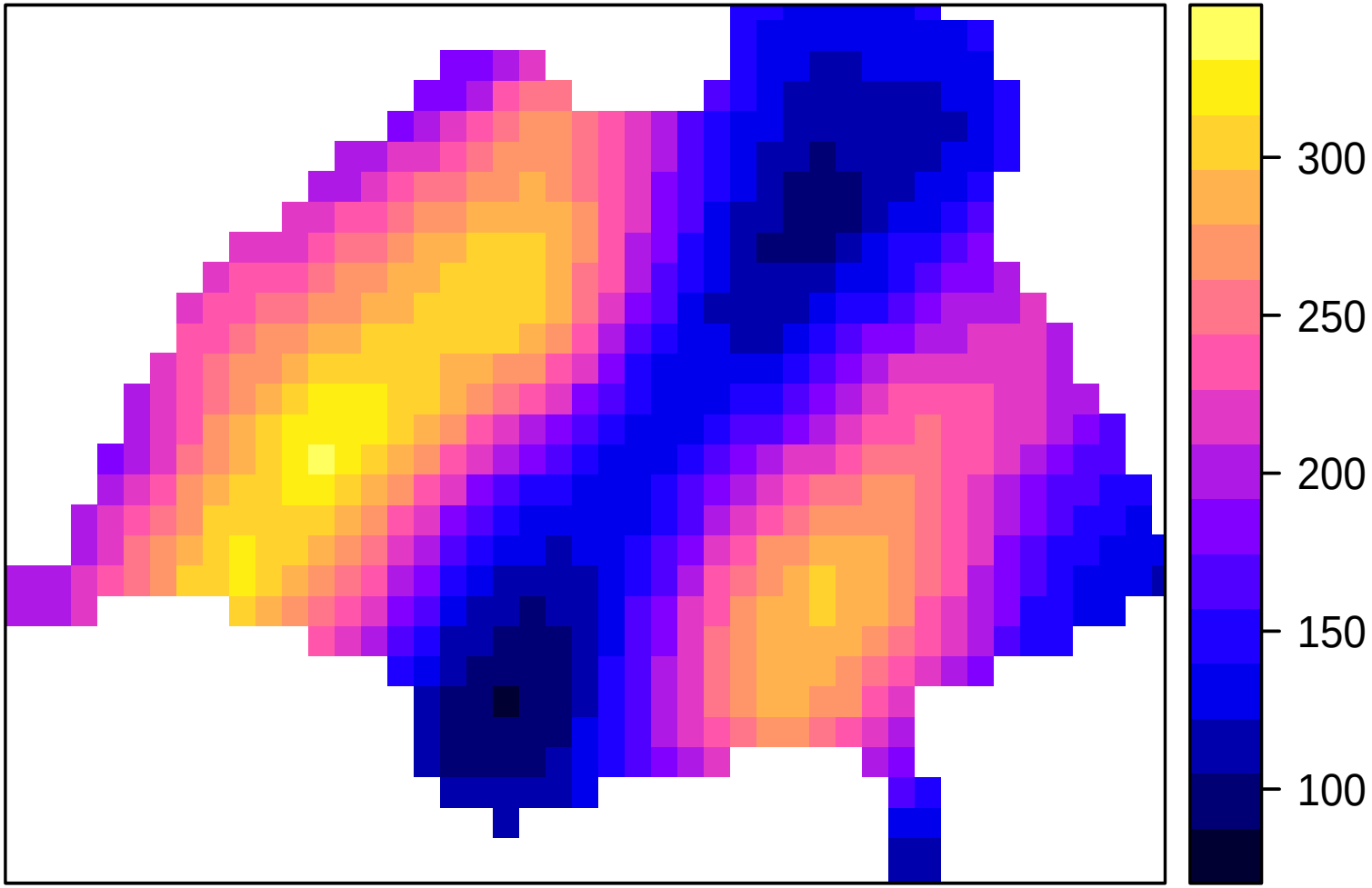
high correl only at short distance

Kriging, shorter range correlation

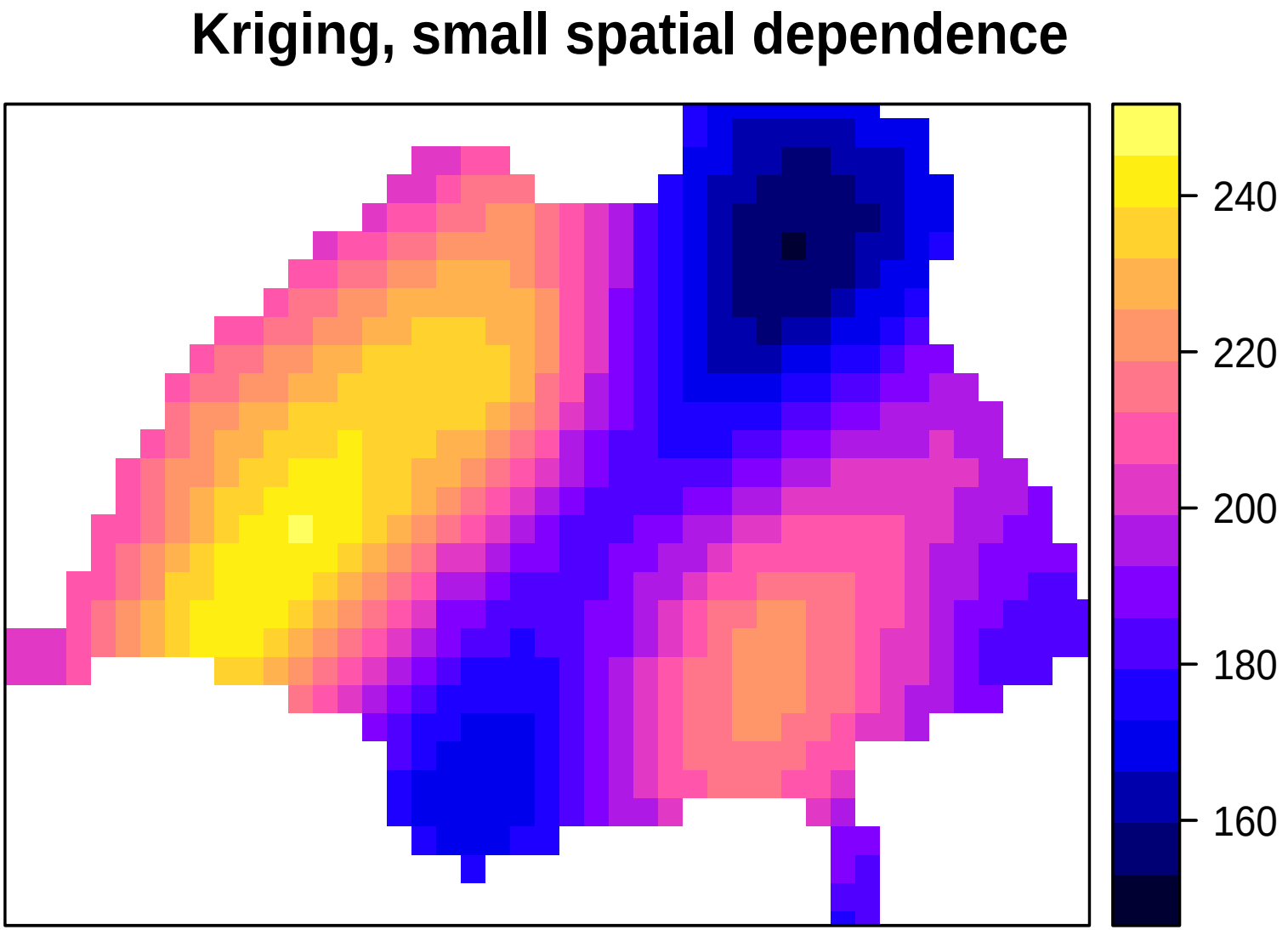


Swiss rainfall

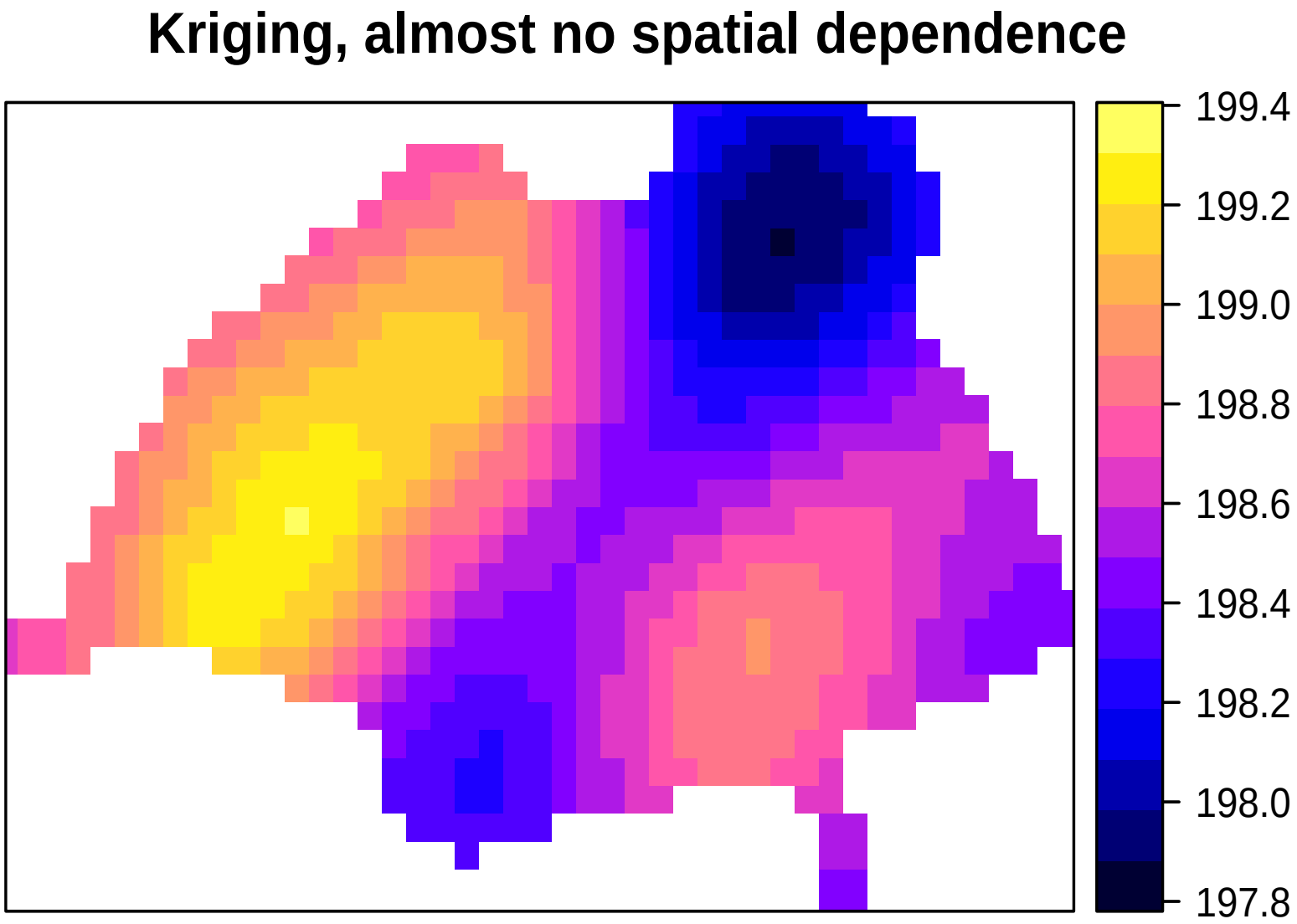
Kriging, less spatial dependence



Swiss rainfall



Swiss rainfall



Universal Kriging

Trend: $Y = X\beta + \varepsilon$ (indep.)

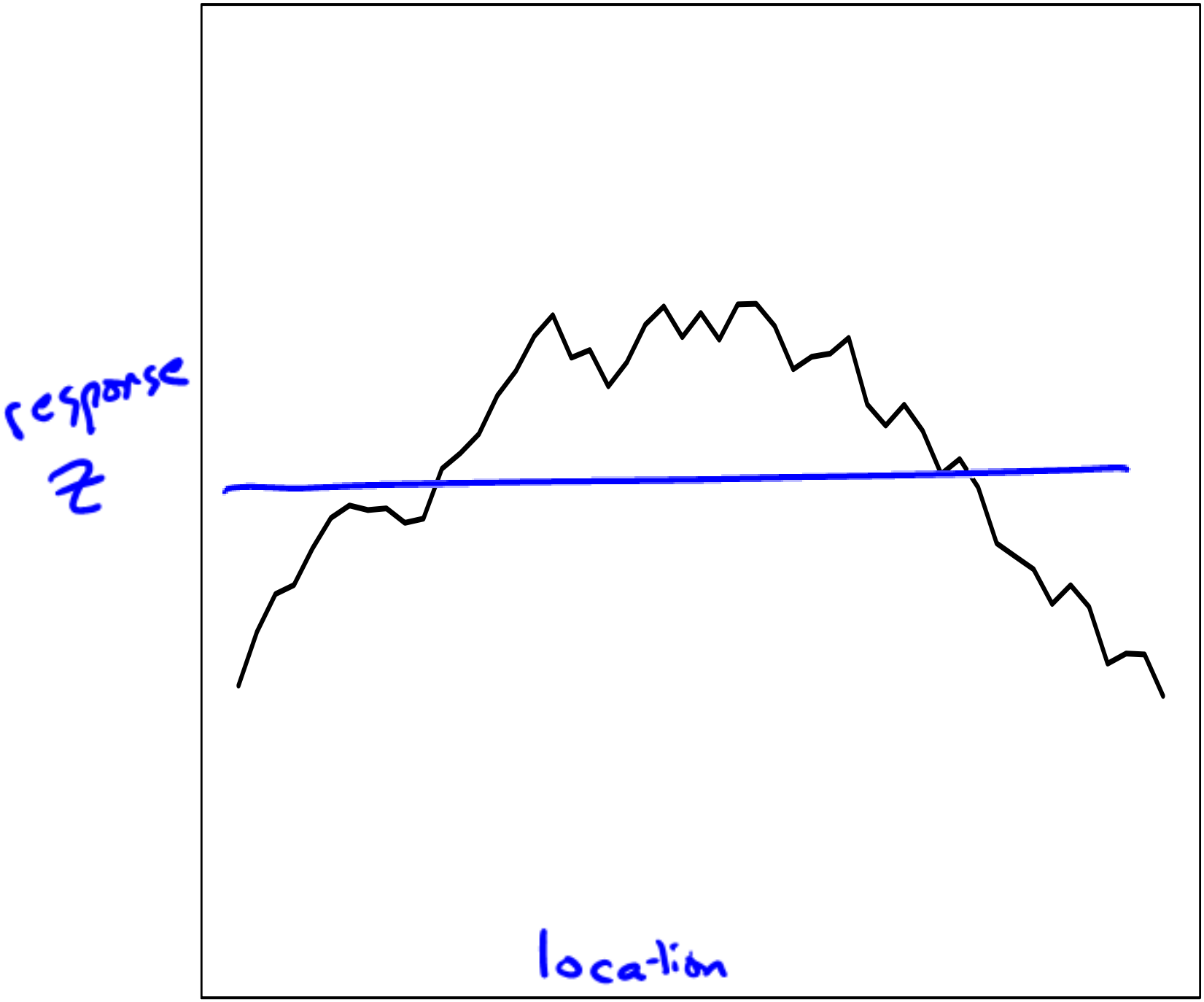
- generalize O.K. to any regression model for local mean (trend / spatial)
- model: $\boldsymbol{Z(s)} = \boldsymbol{X}(s)\beta + \epsilon(s)$ — correlated errors
- i.e. trend + random variation
  - No unique decomposition
  - Generally consider trend as fixed, repeatable, pattern
  - and random variation to be non-repeatable pattern
- Measure Z at 50 spatial locations. What is the sample size?

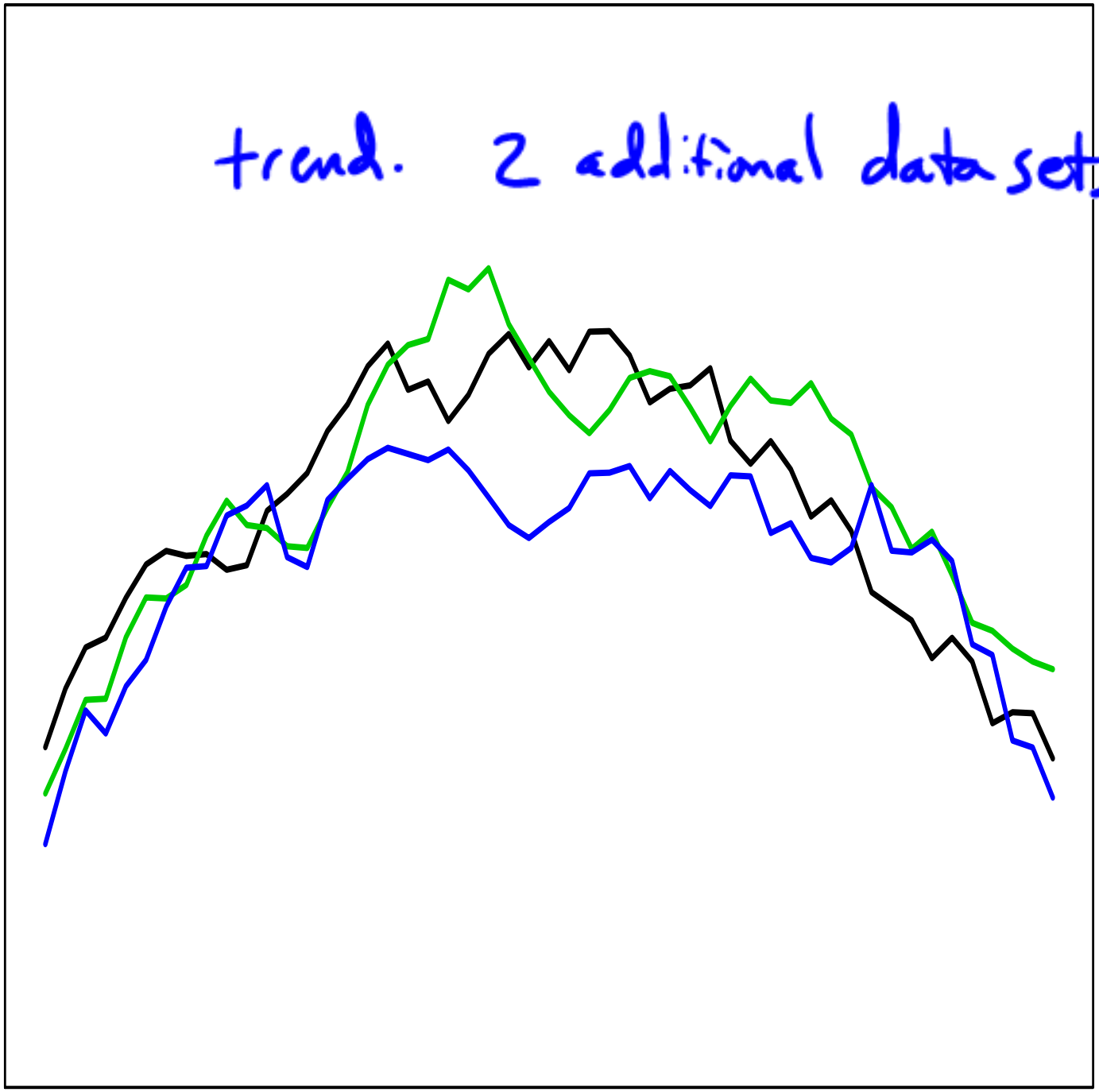
indep $N = 50$.

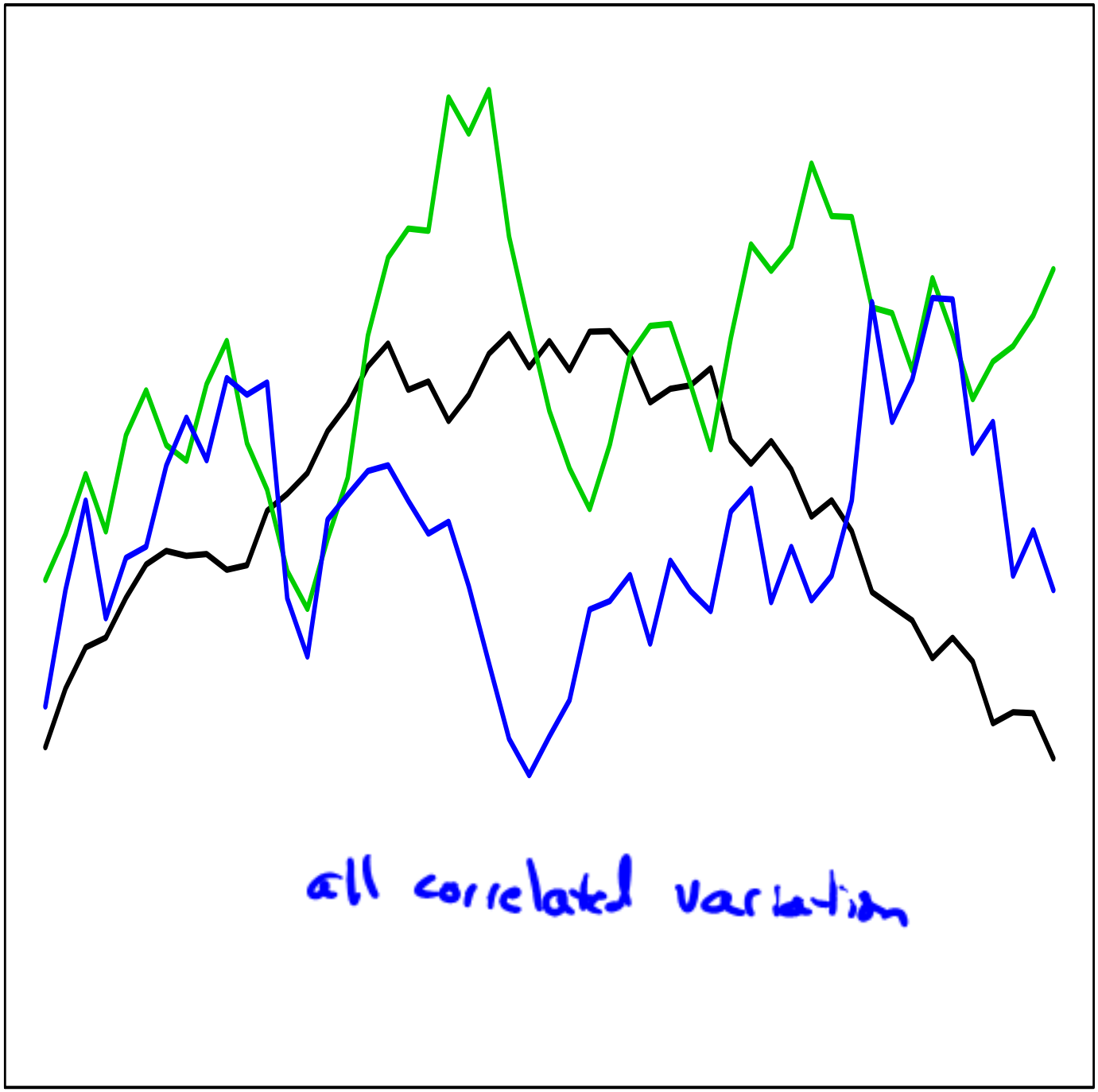
when spatially correl. $N = ($

Universal Kriging

- generalize O.K. to any regression model
- model: $\boldsymbol{Z(s)} = \boldsymbol{X}(s)\boldsymbol{\beta} + \varepsilon(s)$
- i.e. trend + random variation
  - No unique decomposition
  - Generally consider trend as fixed, repeatable, pattern
  - and random variation to be non-repeatable pattern
- Measure Z at 50 spatial locations. Q: What is the sample size?
- A: ONE. You have one realization of that spatial pattern
- Makes it very difficult to distinguish fixed and random components
- Operationally:
  - trend is the variability that can be predicted by $\boldsymbol{X(s)}$
  - random variation is that which can not
- Choice of $\boldsymbol{X(s)}$ is really important!


response
z
location


trend. 2 additional data sets.


all correlated variation

Universal Kriging

- notice that spatial variation accounts for lack of fit to trend model
  - Two competing explanations
  - Defer discussion until we talk about spatial linear models
- Should be able to anticipate the predictor:

$$P(\boldsymbol{s}_0) = \boldsymbol{X}(s)\hat{\beta}_{GLS} + \lambda\left(\boldsymbol{Z}(\boldsymbol{s}) - \boldsymbol{X}(s)\hat{\beta}_{GLS}\right)$$

- and the prediction variance:

$$\sigma^2(\boldsymbol{s}_0) = \sigma^2 - \boldsymbol{\sigma}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\sigma} + \text{term for Var } \boldsymbol{X}(s)\hat{\beta}$$

- the term for Var $\boldsymbol{X}(s)\hat{\beta}$ is complicated, not too informative

$$\hat{\beta}_{GLS} = (\boldsymbol{X}(s)'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(s))^{-1}\boldsymbol{X}(s)'\boldsymbol{\Sigma}^{-1}\boldsymbol{Z}(\boldsymbol{s})$$

Comparison of spatial prediction methods

- Inverse distance weighting
  - more weight to nearby locs
  - wts relative to other nearby locs
  - if no other nearby locs, will still average the more distant locs
  - no easy way to estimate uncertainty in prediction
- Trend surfaces
  - depend on specified model form
  - model is a global model
  - splines based on global est of smoothing param.
    - although there are local extensions
  - estimate doesn't depend on number of nearby locs

choose power.

Comparison of spatial prediction methods

- Kriging:
  - based on correlations among observations
  - estimated from global properties
  - big advantage: estimate depends on number of nearby locs
    - nearby points: prediction more like the local ave.
    - no nearby points: prediction more like the global ave.
  - and data determines how smooth
  - theory: best predictor
    - my experience: not compelling because assumptions never met

Σ amongst obs
σ pred location to obs.

Sand G: Schabenberger and Gotway