Sparse Linear Models

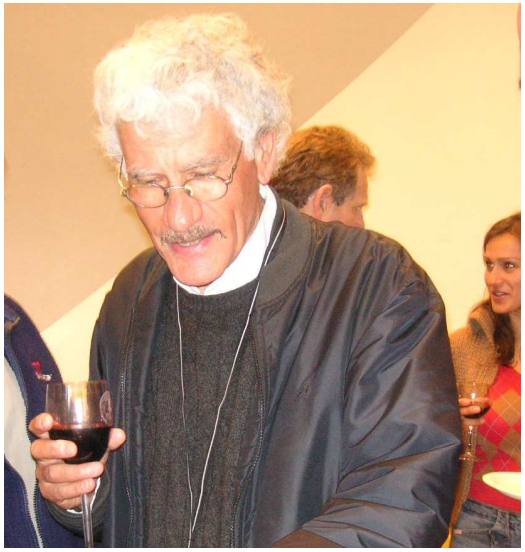
Trevor Hastie

Stanford University

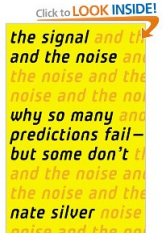
PIMS Public Lecture

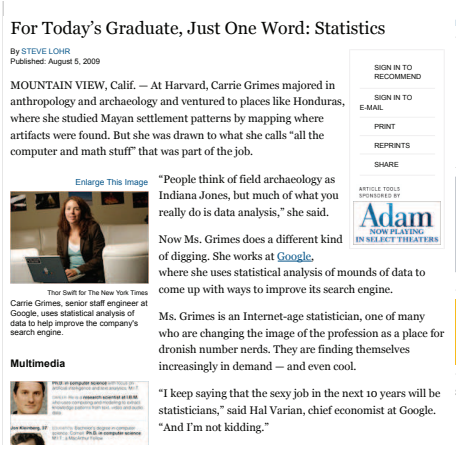
Year of Statistics 2013

joint work with Jerome Friedman, Rob Tibshirani and Noah Simon



Year of Statistics





For Today's Graduate, Just One Word: Statistics

By STEVE LOHR
Published: August 5, 2009

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Thor Swift for The New York Times
Carrie Grimes, senior staff engineer at Google, uses statistical analysis of data to help improve the company's search engine.

"People think of field archaeology as Indiana Jones, but much of what you really do is data analysis," she said.

Now Ms. Grimes does a different kind of digging. She works at Google, where she uses statistical analysis of mounds of data to come up with ways to improve its search engine.

Ms. Grimes is an Internet-age statistician, one of many who are changing the image of the profession as a place for dronish number nerds. They are finding themselves increasingly in demand — and even cool.

"I keep saying that the sexy job in the next 10 years will be statisticians," said Hal Varian, chief economist at Google. "And I'm not kidding."

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Statistics in the news

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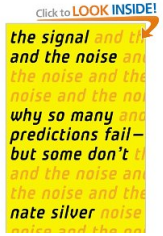
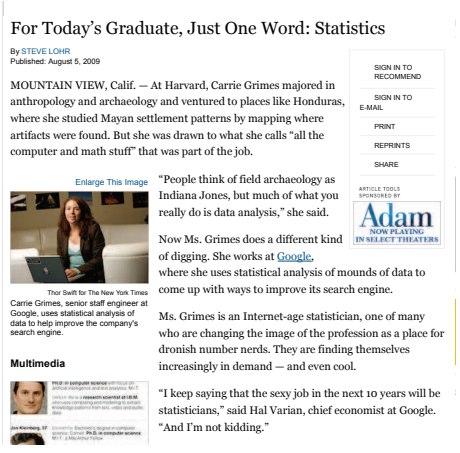
There has never been a better time to be a statistician.

Year of Statistics





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Nerds rule!

Linear Models for Wide Data

As datasets grow *wide*—i.e. many more features than samples—the linear model has regained favor as the tool of choice.

Document classification: bag-of-words easily leads to $p = 20K$ features and $N = 5K$ document samples. Much more if bigrams, trigrams etc, or documents from Facebook, Google, Yahoo!

Genomics, microarray studies: $p = 40K$ genes are measured for each of $N = 300$ subjects.

Genome-wide association studies: $p =$1–2M SNPs measured for $N = 2000$ case-control subjects.

In examples like these we tend to use linear models — e.g. linear regression, logistic regression, Cox model. Since $p \gg N$, we cannot fit these models using standard approaches.

Forms of Regularization

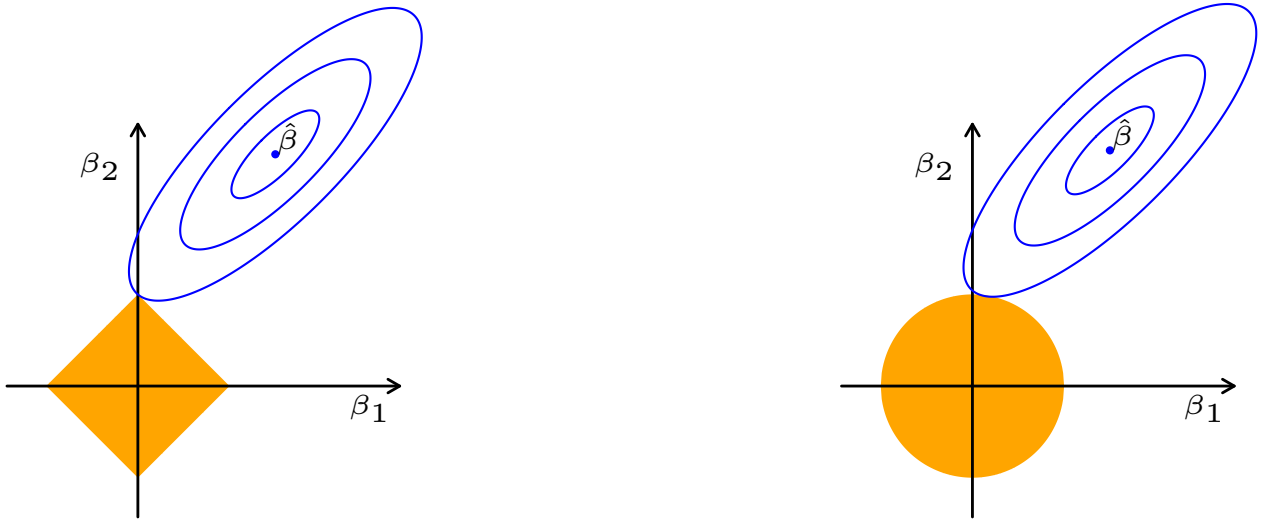
We cannot fit linear models with $p > N$ without some constraints. Common approaches are

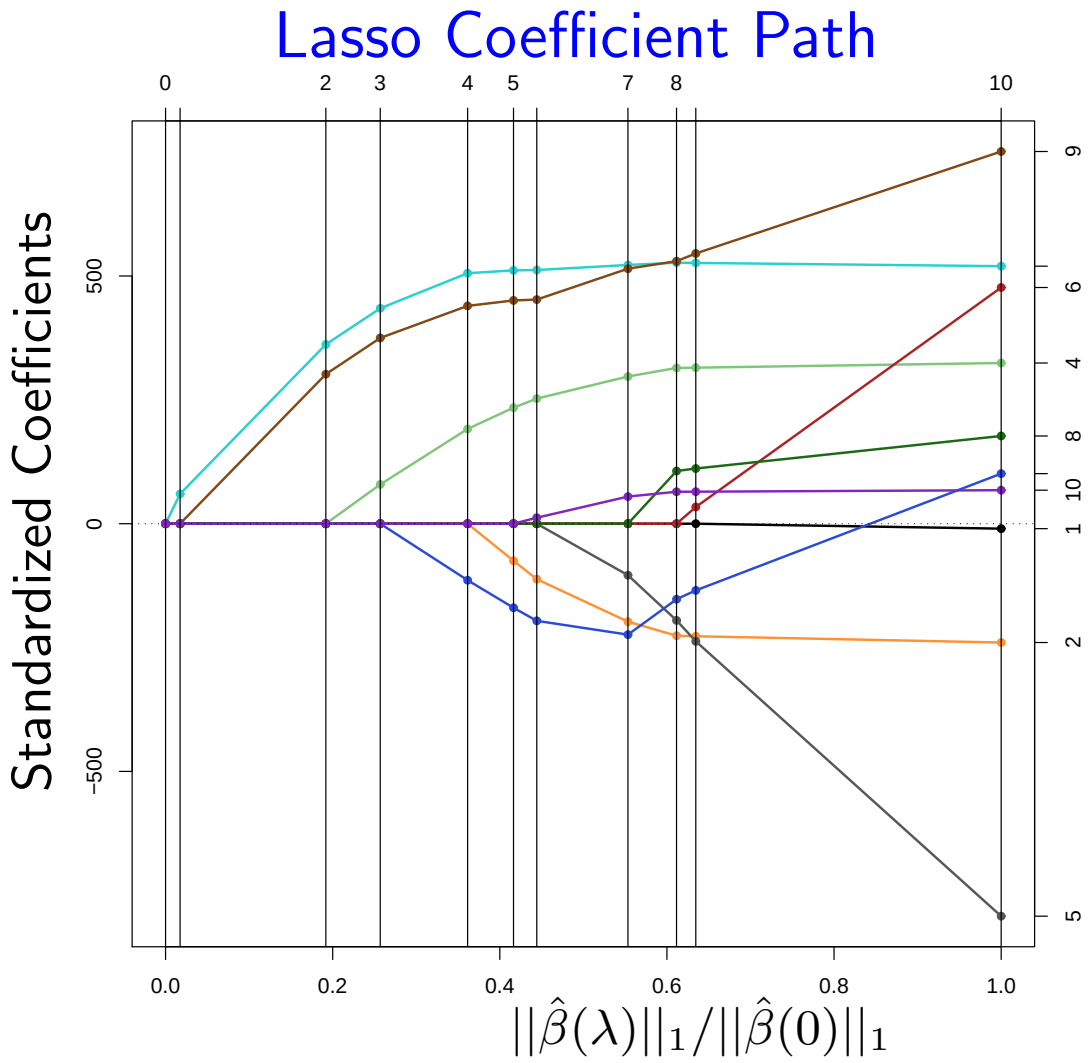
Forward stepwise adds variables one at a time and stops when overfitting is detected. Regained popularity for $p \gg N$, since it is the only feasible method among it's subset cousins (backward stepwise, best-subsets).

Ridge regression fits the model subject to constraint $\sum_{j=1}^{p} \beta_j^2 \leq t$. Shrinks coefficients toward zero, and hence controls variance. Allows linear models with arbitrary size p to be fit, although coefficients always in row-space of X.

Lasso regression (Tibshirani, 1995) fits the model subject to constraint $\sum_{j=1}^{p} |\beta_j| \leq t$.

Lasso does variable selection and shrinkage, while ridge only shrinks.

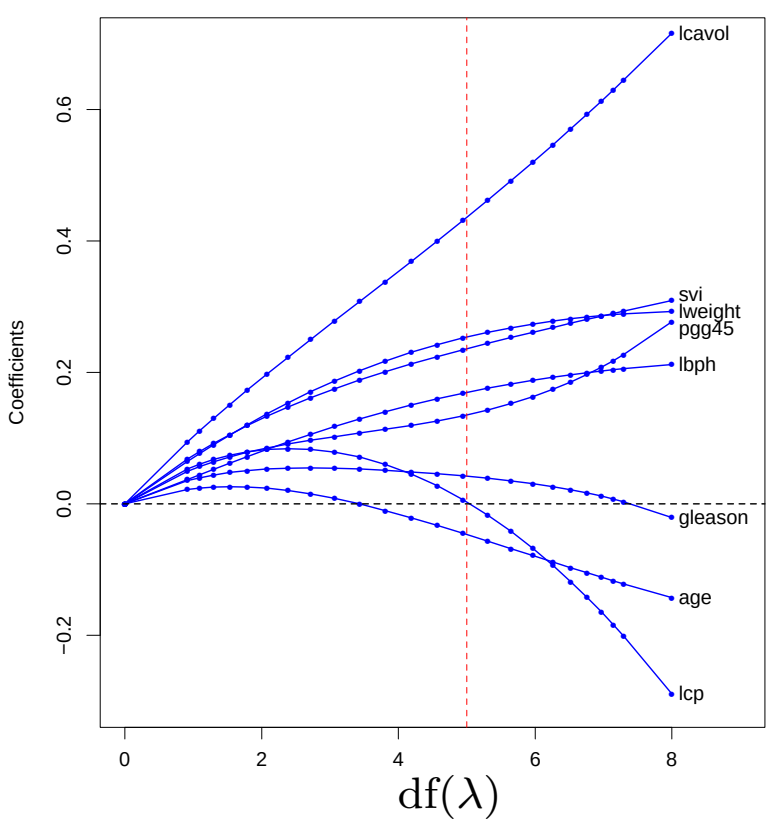


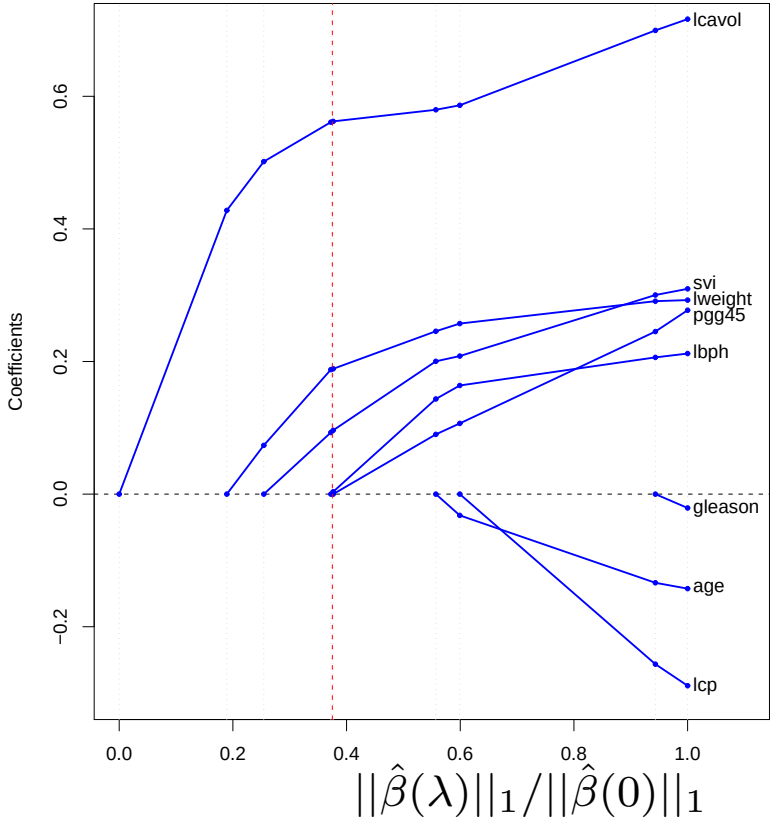


$$\text{Lasso: } \hat{\beta}(\lambda) = \text{argmin}_\beta \frac{1}{N} \sum_{i=1}^{N} (y_i - \beta_0 - x_i^T \beta)^2 + \lambda ||\beta||_1$$

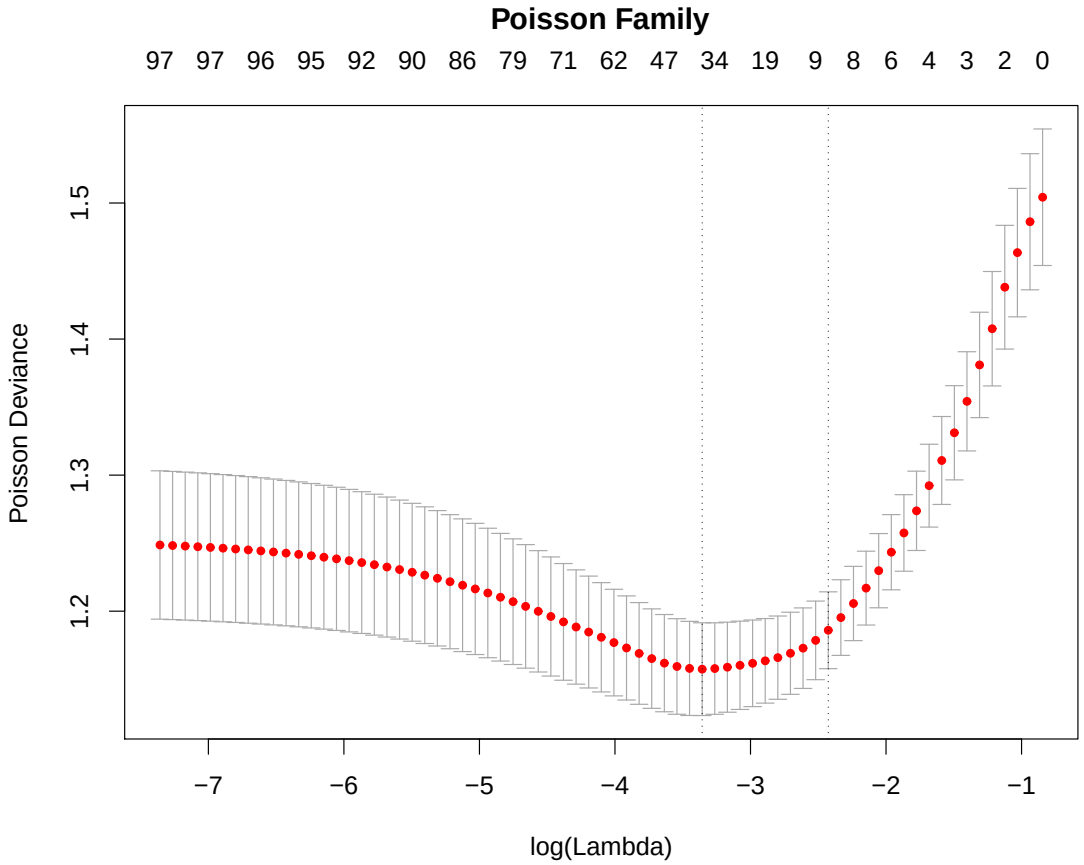
fit using LARS package in R (Efron, Hastie, Johnstone, Tibshirani 2002)

Ridge versus Lasso





Cross Validation to select λ



K-fold cross-validation is easy and fast. Here K=10, and the true model had 10 out of 100 nonzero coefficients.

History of Path Algorithms

Efficient path algorithms for $\hat{\beta}(\lambda)$ allow for easy and exact cross-validation and model selection.

- In 2001 the LARS algorithm (Efron et al) provides a way to compute the entire lasso coefficient path efficiently at the cost of a full least-squares fit.
- 2001 – 2008: path algorithms pop up for a wide variety of related problems: Group lasso (Yuan & Lin 2006), support-vector machine (Hastie, Rosset, Tibshirani & Zhu 2004), elastic net (Zou & Hastie 2004), quantile regression (Li & Zhu, 2007), logistic regression and glms (Park & Hastie, 2007), Dantzig selector (James & Radchenko 2008), ...
- Many of these do not enjoy the piecewise-linearity of LARS, and seize up on very large problems.

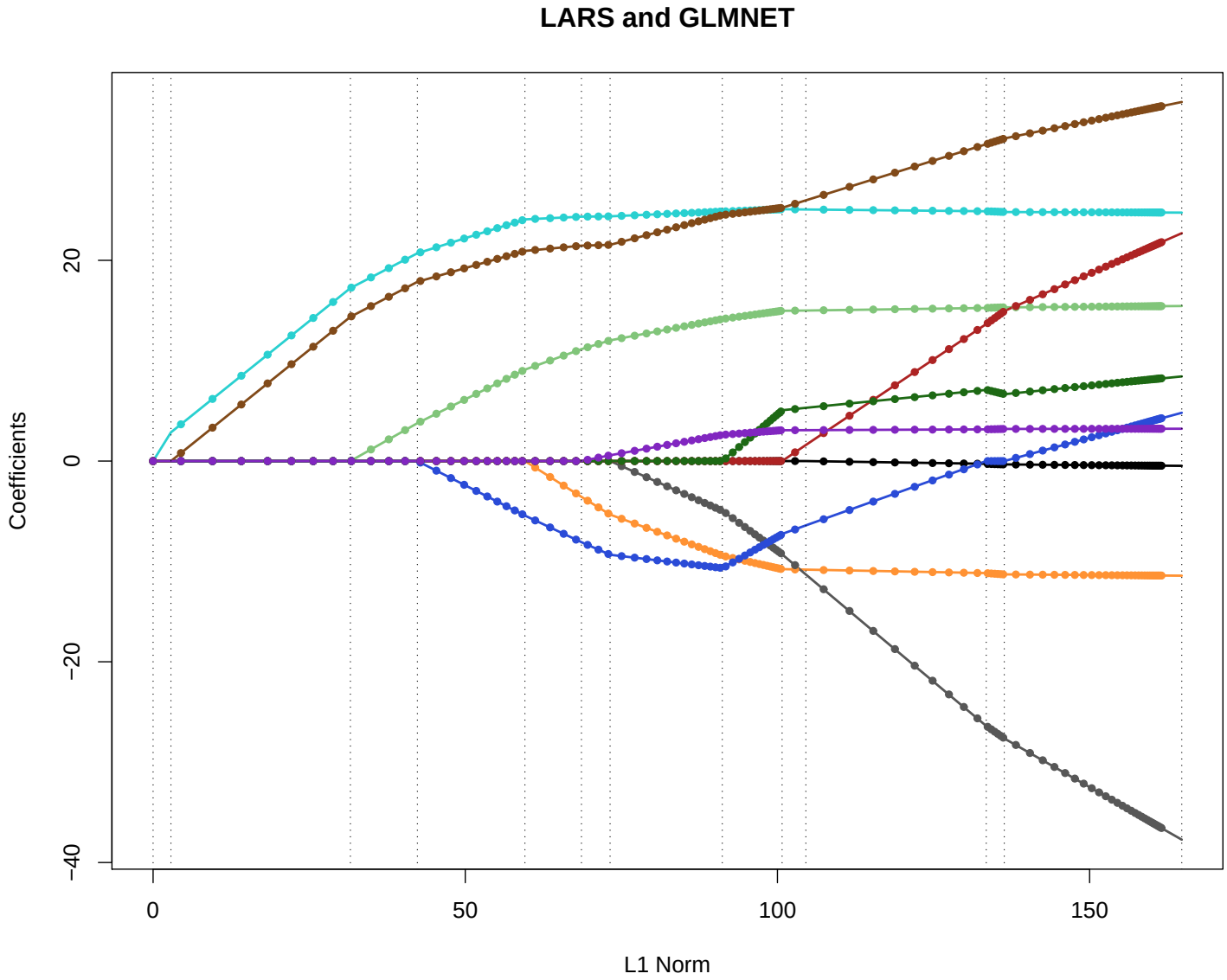
GLMNET and coordinate descent

- Solve the lasso problem by coordinate descent: optimize each parameter separately, holding all the others fixed. Updates are trivial. Cycle around till coefficients stabilize.
- Do this on a grid of λ values, from λ_{max} down to λ_{min} (uniform on log scale), using warms starts.
- Can do this with a variety of loss functions and additive penalties.

Coordinate descent achieves dramatic speedups over all competitors, by factors of 10, 100 and more.

Example: Newsgroup data: 11K obs, 778K features (sparse), 100 values λ across entire range, lasso logistic regression; time 29s on Macbook Pro.

References: Friedman, Hastie and Tibshirani 2008 + long list of other who have also worked with coordinate descent.


LARS and GLMNET
Coefficients
20
0
−20
−40
0
50
100
150
L1 Norm

GLMNET package in R

Fits coefficient paths for a variety of different GLMs and the *elastic net* family of penalties.

Some features of `glmnet`:

- Models: linear, logistic, multinomial (grouped or not), Poisson, Cox model, and multiple-response grouped linear.
- Elastic net penalty includes *ridge* and *lasso*, and hybrids in between (more to come)
- *Speed!*
- Can handle large number of variables p. Along with screening rules we can fit GLMs on GWAS scale (more to come)
- Cross-validation functions for all models.
- Can allow for sparse matrix formats for $\mathbf{X}$, and hence massive

problems (eg $N = 11K$, $p = 750K$ logistic regression).

- Can provide lower and upper bounds for each coefficient; eg: positive lasso
- Useful bells and whistles:
  - Offsets — as in GLM, can have part of the linear predictor that is given and not fit. Often used in Poisson models (sampling frame).
  - Penalty strengths — can alter relative strength of penalty on different variables. Zero penalty means a variable is *always in* the model. Useful for adjusting for demographic variables.
  - Observation weights allowed.
  - Can fit no-intercept models
  - Session-wise parameters can be set with new `glmnet.options` command.

Coordinate descent for the lasso

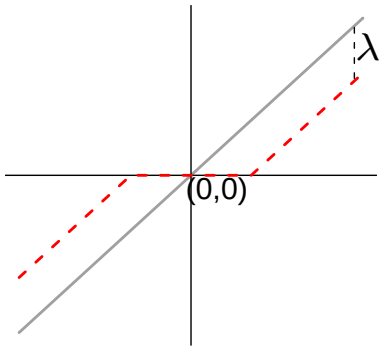
$$\min_\beta \frac{1}{2N}\sum_{i=1}^N (y_i - \sum_{j=1}^p x_{ij}\beta_j)^2 + \lambda\sum_{j=1}^p |\beta_j|$$

Suppose the p predictors and response are standardized to have mean zero and variance 1. Initialize all the $\beta_j = 0$.

Cycle over $j = 1, 2, \ldots, p, 1, 2, \ldots$ till convergence:

- Compute the partial residuals $r_{ij} = y_i - \sum_{k\neq j} x_{ik}\beta_k$.
- Compute the simple least squares coefficient of these residuals on jth predictor: $\beta_j^* = \frac{1}{N}\sum_{i=1}^N x_{ij}r_{ij}$
- Update β_j by *soft-thresholding*:

$$\begin{aligned}\beta_j &\leftarrow S(\beta_j^*, \lambda)\\ &= \text{sign}(\beta_j^*)(|\beta_j^*| - \lambda)_+\end{aligned}$$



Elastic-net penalty family

Family of convex penalties proposed in Zou and Hastie (2005) for $p \gg N$ situations, where predictors are correlated in groups.

$$\min_\beta \frac{1}{2N}\sum_{i=1}^N (y_i - \sum_{j=1}^p x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^p P_\alpha(\beta_j)$$

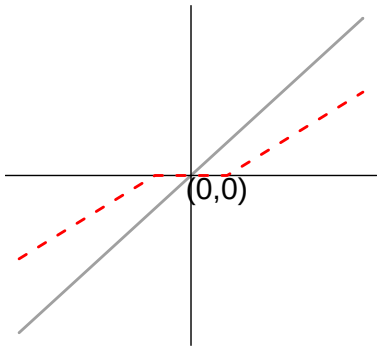
$$\text{with } P_\alpha(\beta_j) = \frac{1}{2}(1-\alpha)\beta_j^2 + \alpha|\beta_j|.$$

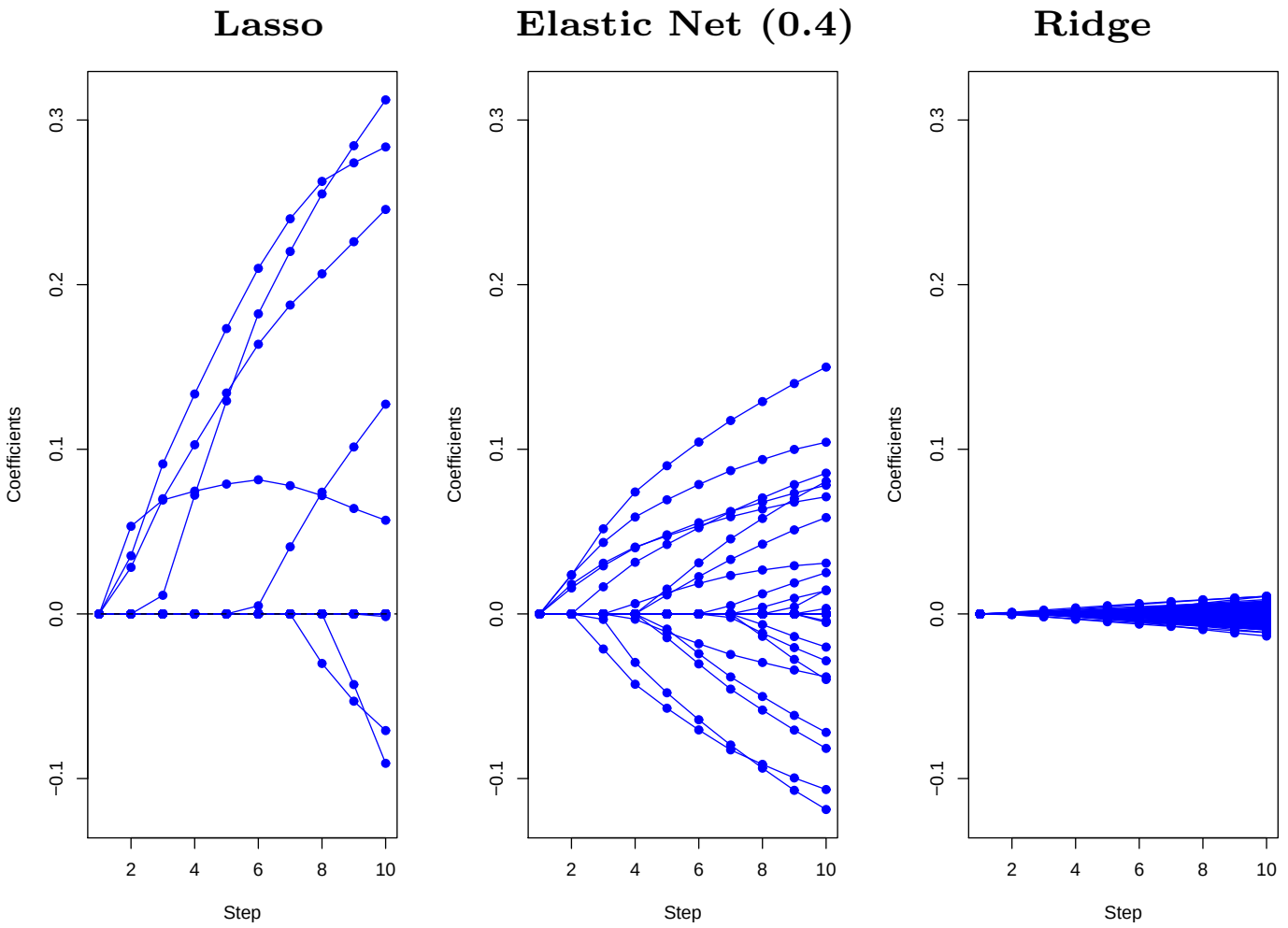
α creates a compromise between the *lasso* and *ridge*.

Coordinate update is now

$$\beta_j \leftarrow \frac{S(\beta_j^*,\ \lambda\alpha)}{1+\lambda(1-\alpha)}$$

where $\beta_j^* = \frac{1}{N}\sum_{i=1}^N x_{ij}r_{ij}$ as before.





Leukemia Data, Logistic, N=72, p=3571, first 10 steps shown

Screening Rules

Logistic regression for GWAS: $p \sim$ million, $N = 2000$
(Wu et al, 2009)

- Compute $|\langle x_j, y - \bar{y}\rangle|$ for each Snp $j = 1, 2, \ldots, 10^6$, where $\bar{y}$ is the mean of (binary) y.
  Note: the largest of these is λ_{max} — smallest value of λ for which all coefficients are zero.
- Fit lasso logistic regression path using only largest 1000 (typically fit models of size around 20 or 30 in GWAS)
- Simple confirmations check that omitted Snps would not have entered the model.

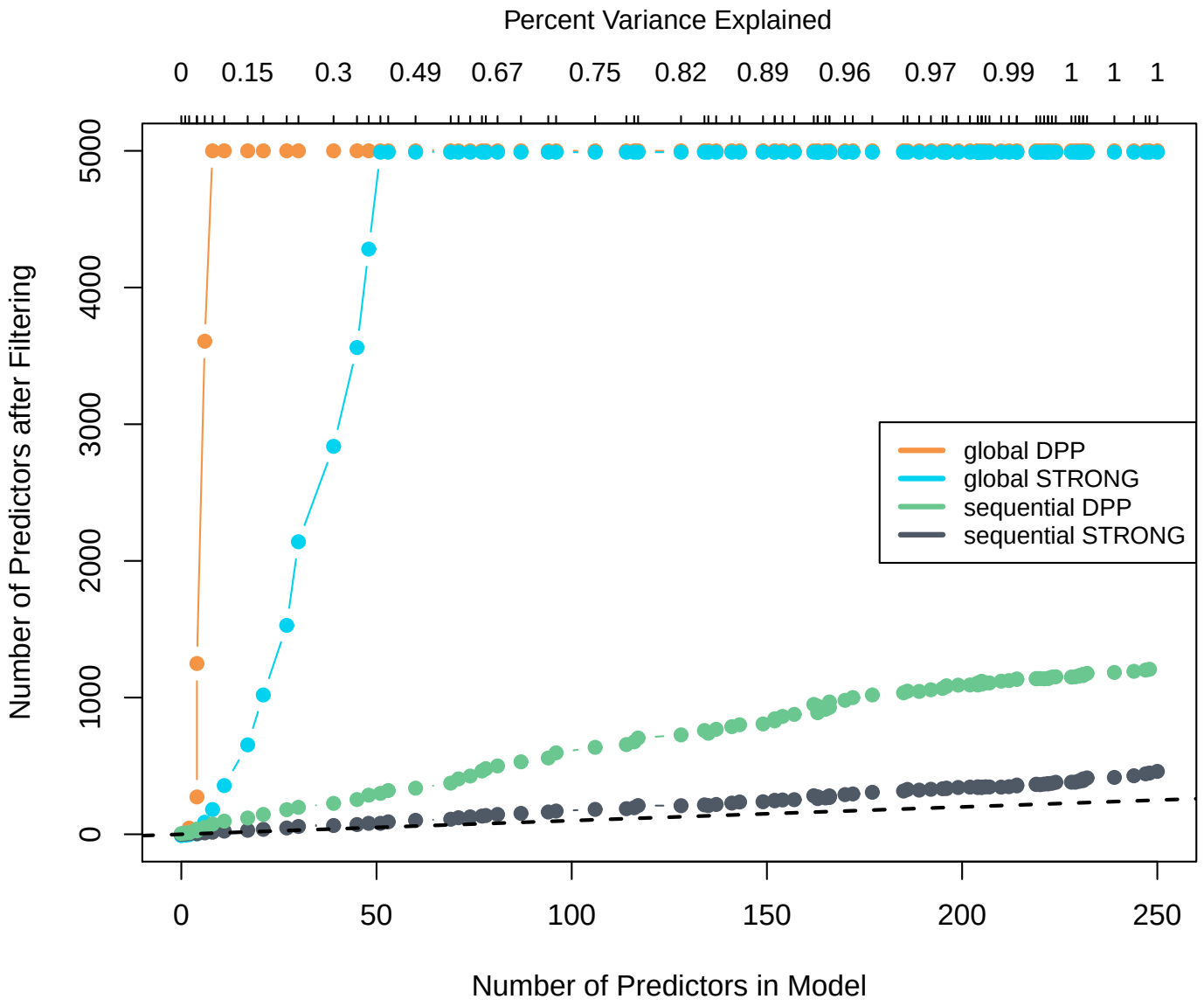
Safe and Strong Rules

- El Ghaoui et al (2010), improved by Wang et al (2012) propose SAFE rules for Lasso for screening predictors — can be quite conservative.
- Tibshirani et al (2012) improve these using STRONG screening rules.

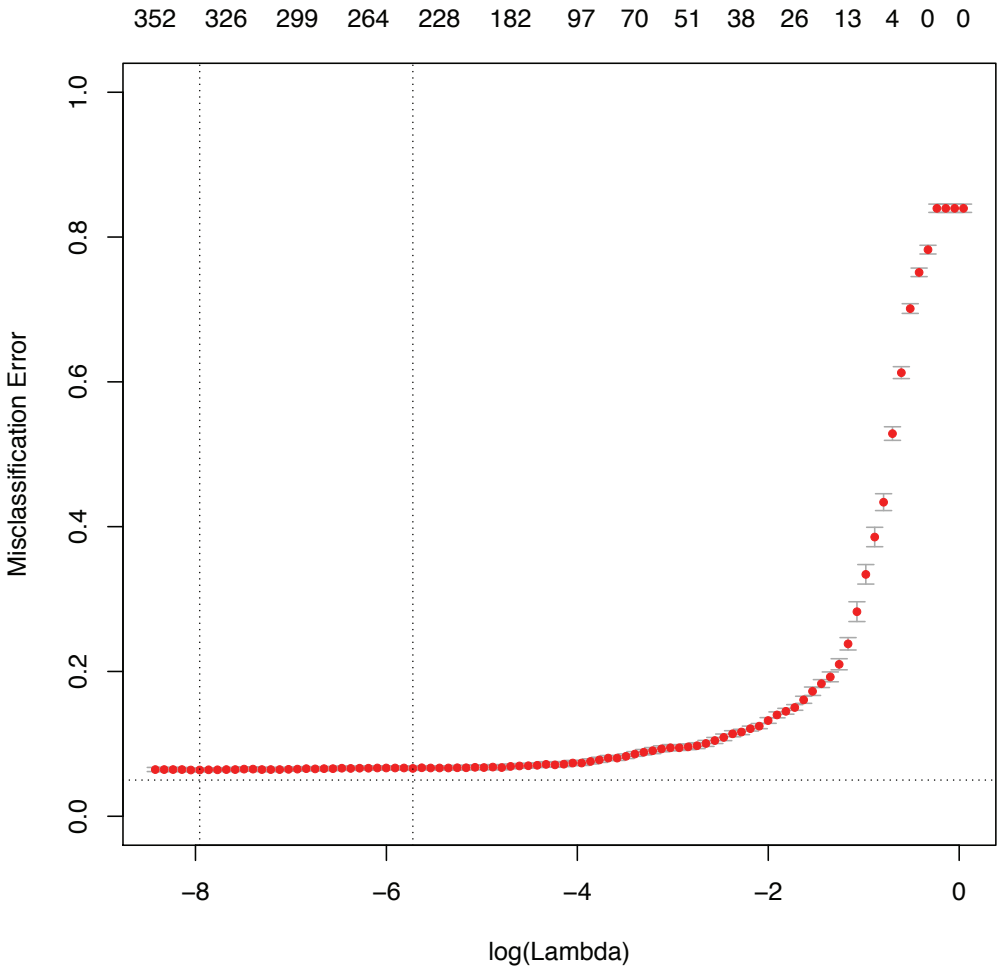
  Suppose fit at λ_ℓ is $\mathbf{X}\hat{\beta}(\lambda_\ell)$, and we want to compute the fit at $\lambda_{\ell+1} < \lambda_\ell$. Note: $|\langle \mathbf{x}_j, \mathbf{y} - \mathbf{X}\hat{\beta}(\lambda_\ell)\rangle| = \lambda_\ell \ \forall j \in \mathcal{A}$. ,
  $\leq \lambda_\ell \ \forall j \notin \mathcal{A}$.
  Strong rules only consider set

$$\left\{ j : |\langle \mathbf{x}_j, \mathbf{y} - \mathbf{X}\hat{\beta}(\lambda_\ell)\rangle| > \lambda_{\ell+1} - (\lambda_\ell - \lambda_{\ell+1}) \right\}$$

  GLMNET screens at every λ step, and after convergence, checks if any violations.


Percent Variance Explained
0
0.15
0.3
0.49
0.67
0.75
0.82
0.89
0.96
0.97
0.99
1
1
1
Number of Predictors after Filtering
0
1000
2000
3000
4000
5000
0
50
100
150
200
250
Number of Predictors in Model
global DPP
global STRONG
sequential DPP
sequential STRONG

Example: multiclass classification



Pathwork® Diagnostics

Microarray classification: tissue of origin

3220 samples

22K genes

17 classes (tissue type)

Multinomial regression model with

$17 \times 22\text{K} = 374\text{K}$ parameters

Elastic-net ($\alpha = 0.25$)

Example: HIV drug resistance

Paper looks at *in vitro* drug resistance of $N = 1057$ HIV-1 isolates to protease and reverse transcriptase mutations. Here we focus on Lamivudine (a Nucleoside RT inhibitor). There are $p = 217$ (binary) mutation variables.

Paper compares 5 different regression methods: decision trees, neural networks, SVM regression, OLS and LAR (lasso).

Genotypic predictors of human immunodeficiency virus type 1 drug resistance

Soo-Yon Rhee, Jonathan Taylor, Gauhar Wadhera, Asa Ben-Hur, Douglas L. Brutlag, and Robert W. Shafer

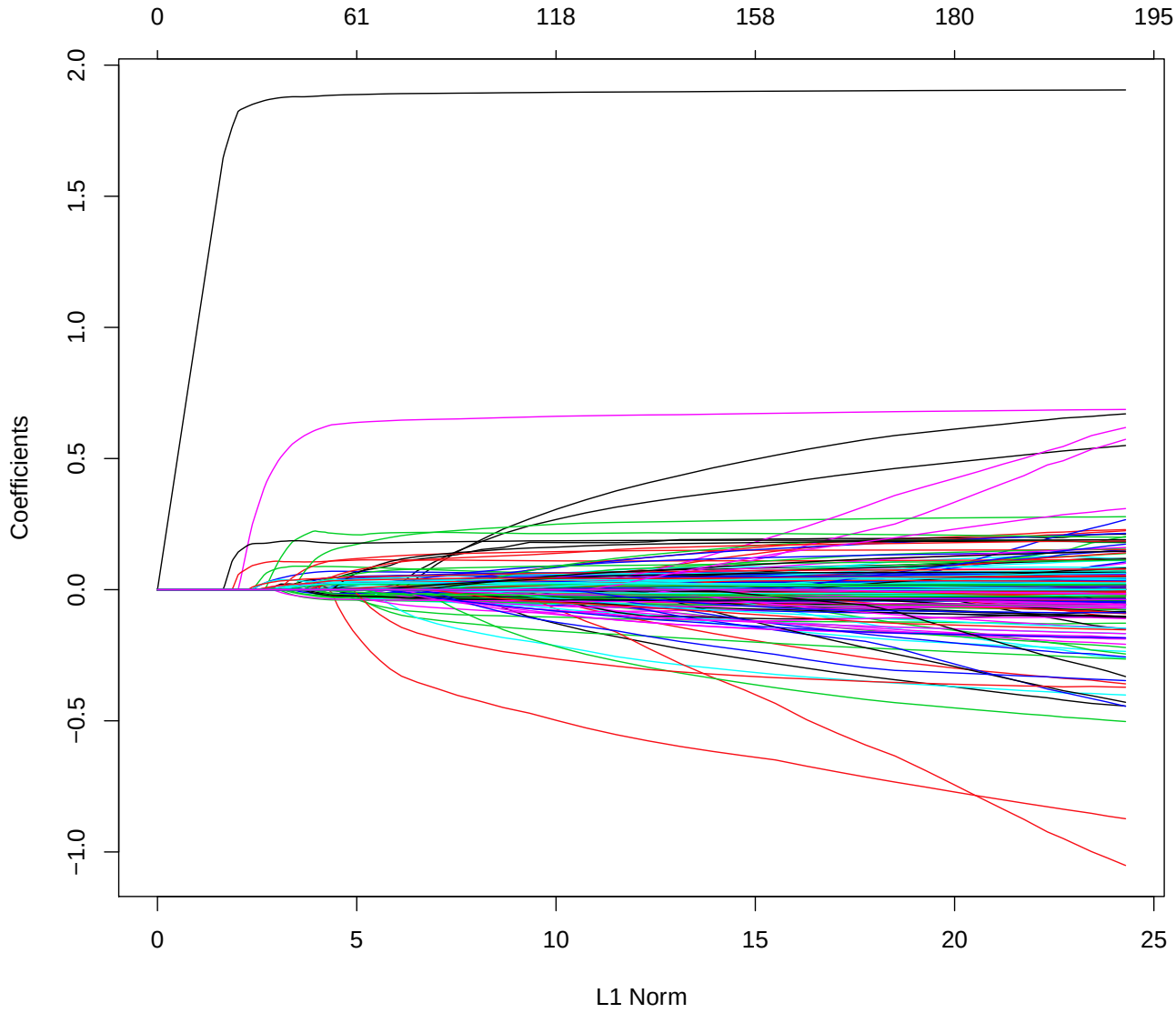
PNAS published online Oct 25, 2006;

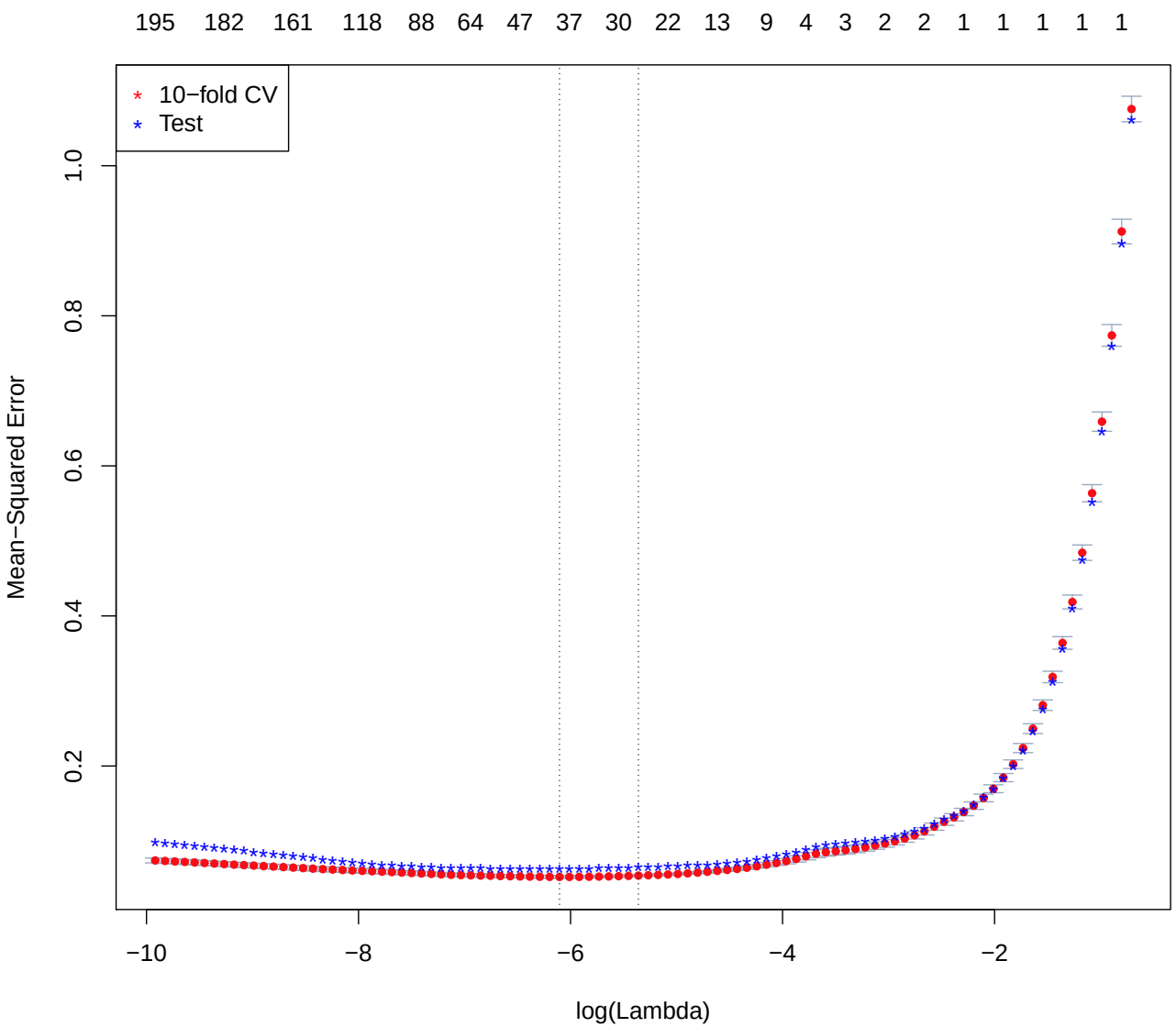
.

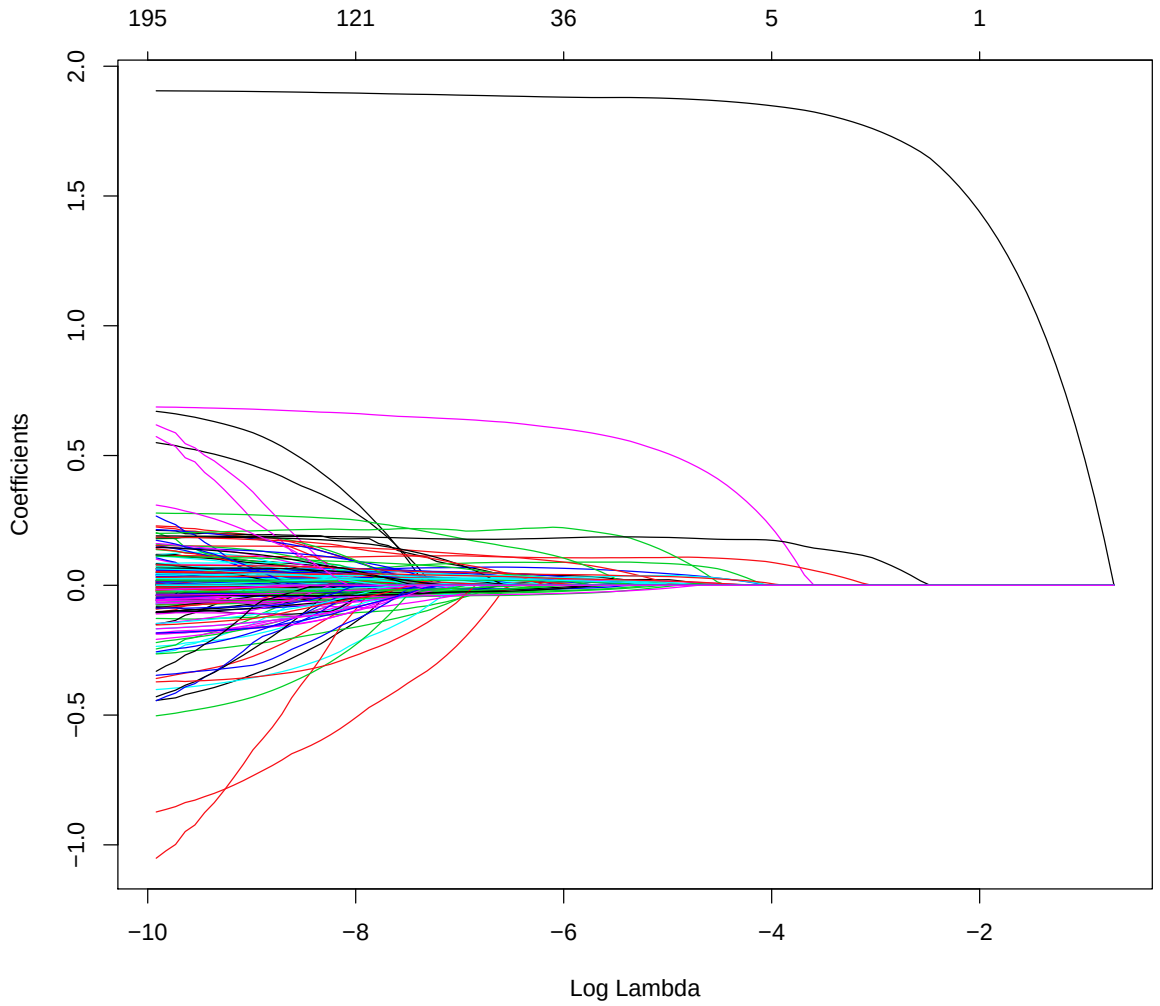
R code for fitting model

```
> require(glmnet)
> fit=glmnet(xtr,ytr,standardize=FALSE)
> plot(fit)

> cv.fit=cv.glmnet(xtr,ytr,standardize=FALSE)
> plot(cv.fit)
>
> mte=predict(fit,xte)
> mte= apply( (mte-yte)^2,2,mean)
> points(log(fit$lambda),mte,col="blue",pch="*")
> legend("topleft",legend=c("10-fold CV","Test"),
          pch="*",col=c("red","blue"))
```


0
61
118
158
180
195
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
Coefficients
0
5
10
15
20
25
L1 Norm


195 182 161 118 88 64 47 37 30 22 13 9 4 3 2 2 1 1 1 1 1
10−fold CV
Test
Mean−Squared Error
0.2
0.4
0.6
0.8
1.0
−10
−8
−6
−4
−2
log(Lambda)

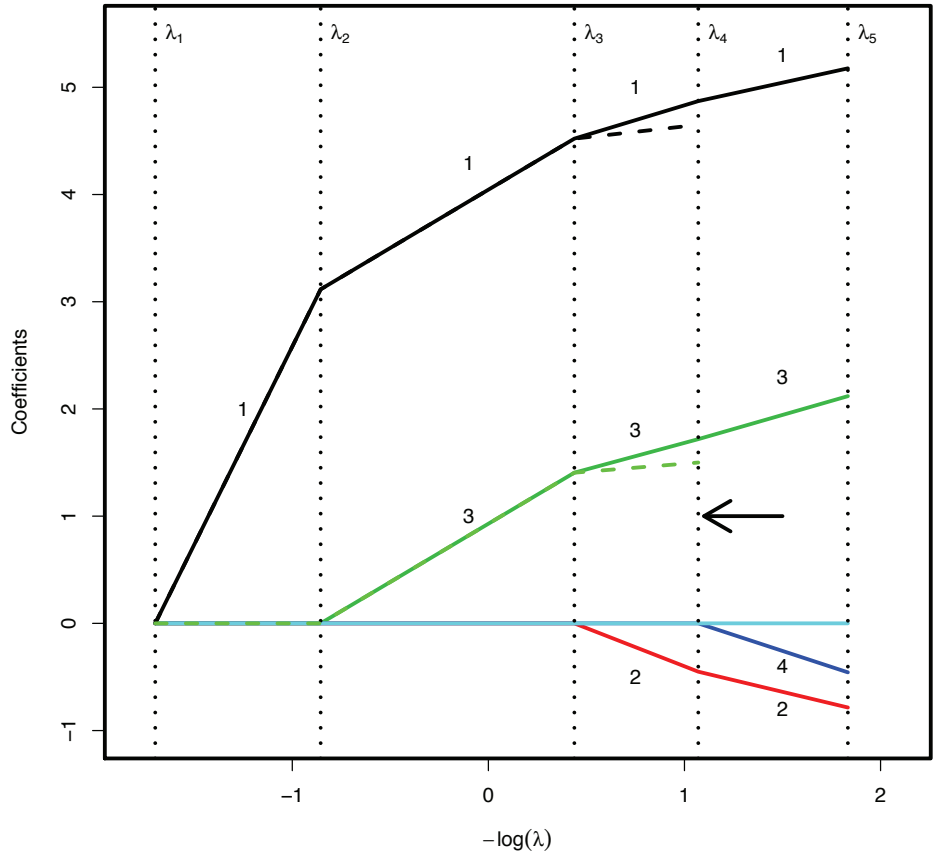



```
> plot(fit,xvar="lambda")
```

Inference?

- Can become Bayesian! Lasso penalty corresponds to Laplacian prior. However, need priors for everything, including λ (variance ratio). Easier to bootstrap, with similar results.
- Covariance Test. Very exciting new developments here: "A Significance Test for the Lasso" — Lockhart, Taylor, Ryan Tibshirani and Rob Tibshirani (2013)
  - We learned from the LARS project that at each step (knot) we spend one additional degree of freedom.
  - This test delivers a test statistic that is Exp(1) under the null hypothesis that the included variable is noise, but all the earlier variables are signal.

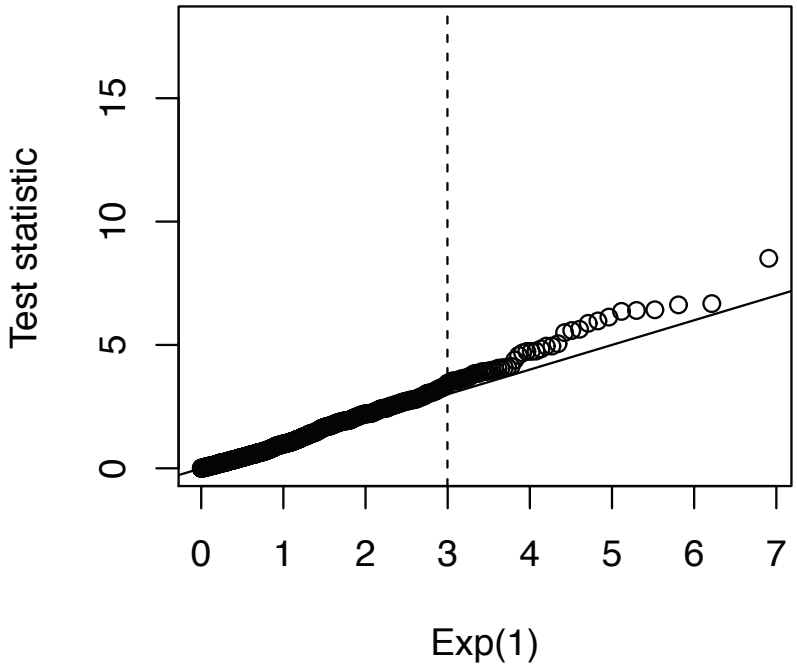
- Suppose we want a p-value for predictor 2, entering at step 3.
- Compute "covariance" at λ_4: $\langle \mathbf{y}, \mathbf{X}\hat{\beta}(\lambda_4)\rangle$
- Drop X_2, yielding active set A; refit at λ_4, and compute covariance at λ_4: $\langle \mathbf{y}, \mathbf{X}_{\mathcal{A}}\hat{\beta}_{\mathcal{A}}(\lambda_4)\rangle$



Covariance Statistic and Null Distribution

Under the null hypothesis that all signal variables are in the model:

$$\frac{1}{\sigma^2} \cdot \Big(\langle \mathbf{y}, \mathbf{X}\hat{\beta}(\lambda_{j+1}) \rangle - \langle \mathbf{y}, \mathbf{X}_{\mathcal{A}}\hat{\beta}_{\mathcal{A}}(\lambda_{j+1}) \rangle \Big) \to \text{Exp}(1) \text{ as } p, n \to \infty$$



Summary and Generalizations

Many problems have the form

$$\min_{\{\beta_j\}_1^p} \left[R(y, \beta) + \lambda \sum_{j=1}^{p} P_j(\beta_j) \right].$$

- If R and P_j are convex, and R is differentiable, then coordinate descent converges to the solution (Tseng, 1988).
- Often each coordinate step is trivial. E.g. for lasso, it amounts to soft-thresholding, with many steps leaving $\hat{\beta}_j = 0$.
- Decreasing λ slowly means not much cycling is needed.
- Coordinate moves can exploit sparsity.

Other Applications

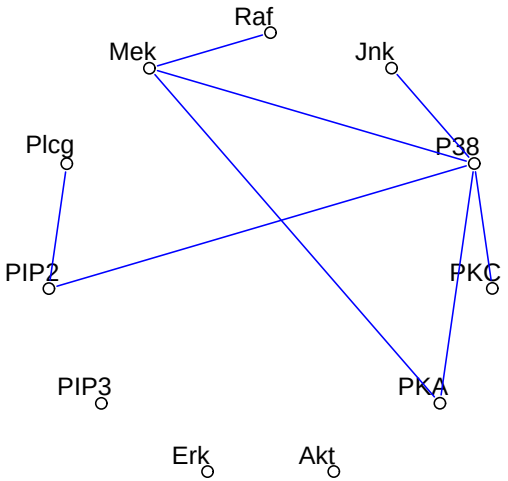
Undirected Graphical Models — learning dependence structure via the lasso. Model the inverse covariance $\mathbf{\Theta}$ in the Gaussian family with L_1 penalties applied to elements.

$$\max_{\mathbf{\Theta}} \log\det \mathbf{\Theta} - \mathrm{Tr}(\mathbf{S\Theta}) - \lambda||\mathbf{\Theta}||_1$$

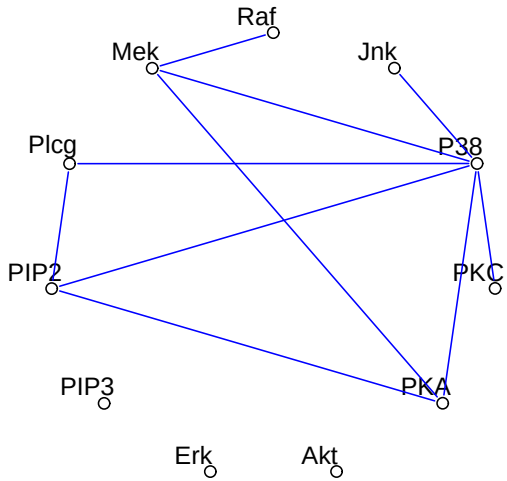
GLASSO: modified block-wise lasso algorithm, which we solve by coordinate descent (FHT 2007). Algorithm is very fast, and solve moderately sparse graphs with 1000 nodes in under a minute.

Example: flow cytometry - $p = 11$ proteins measured in $N = 7466$ cells (Sachs et al 2003) (next page)

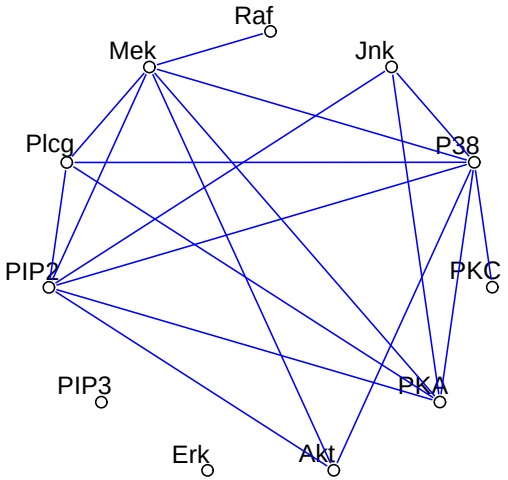
$\lambda = 36$



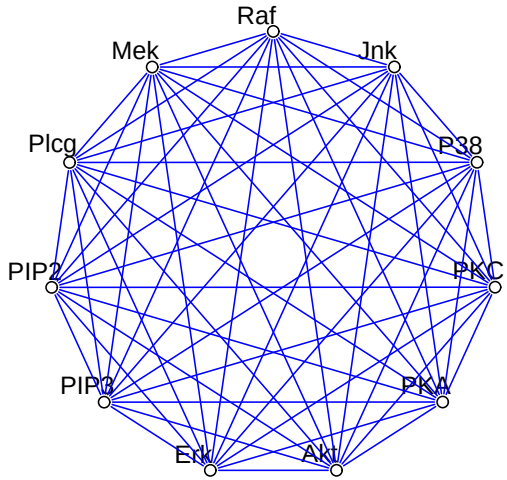
$\lambda = 27$



$\lambda = 7$



$\lambda = 0$



Group Lasso (Yuan and Lin, 2007, Meier, Van de Geer, Buehlmann, 2008) — each term $P_j(\beta_j)$ applies to *sets* of parameters:

$$R(y, \sum_{j=1}^{J} \mathbf{X}_j \beta_j) + \lambda \sum_{j=1}^{J} \gamma_j ||\beta_j||_2.$$

Example: each block represents the levels for a categorical predictor.

- entire groups are zero, or all elements are nonzero.
- γ_j is penalty modifier for group j; $\gamma_j = \|\mathbf{X}_j\|_F$ is good choice.
- Leads to a block-updating form of coordinate descent.
- Strong rules apply here: $\|\mathbf{X}_j^T \mathbf{r}\|_2 > \gamma_j[\lambda_{\ell+1} - (\lambda_\ell - \lambda_{\ell+1})]$

Mixed Graphical Models

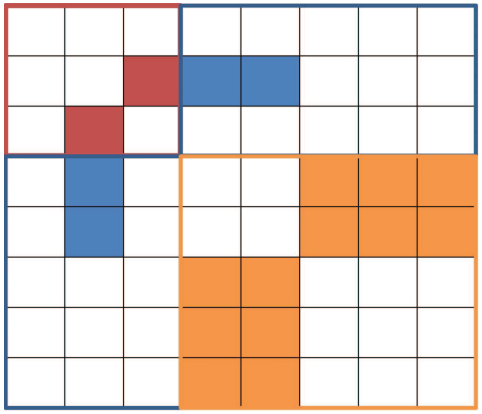
Project with PhD student Jason Lee.
General Markov random field representation, with edge and node potentials.

$$p(x,y;\Theta) \propto \exp\left(\sum_{s=1}^{p}\sum_{t=1}^{p} -\frac{1}{2}\beta_{st}x_s x_t + \sum_{s=1}^{p}\alpha_s x_s + \sum_{s=1}^{p}\sum_{j=1}^{q}\rho_{sj}(y_j)x_s + \sum_{j=1}^{q}\sum_{r=1}^{q}\phi_{rj}(y_r,y_j)\right)$$

- Pseudo likelihood allows simple inference with mixed variables. Conditionals for continuous are Gaussian linear regression models, for categorical are binomial or multinomial logistic regressions.
- Parameters come in symmetric blocks, and the inference should respect this symmetry (next slide)

Mixed Graphical Model: group-lasso penalties

Parameters in blocks. Here we have an interaction between a pair of quantitative variables (red), a 2-level qualitative with a quantitative (blue), and an interaction between the 2 level and a 3 level qualitative.



Maximize a pseudo-likelihood with lasso and group-lasso penalties on parameter blocks.

$$\max_{\Theta} \ell(\Theta) - \lambda \left(\sum_{s=1}^{p} \sum_{t=1}^{s-1} |\beta_{st}| + \sum_{s=1}^{p} \sum_{j=1}^{q} \|\rho_{sj}\|_2 + \sum_{j=1}^{q} \sum_{r=1}^{j-1} \|\phi_{rj}\|_F \right)$$

Solved using proximal Newton algorithm for a decreasing sequence of values for λ [Lee and Hastie, 2013].

Overlap Group Lasso (Jacob et al, 2009) Example: consider the model

$$\eta(X) = X_1\beta_1 + X_1\theta_1 + X_2\theta_2$$

with penalty

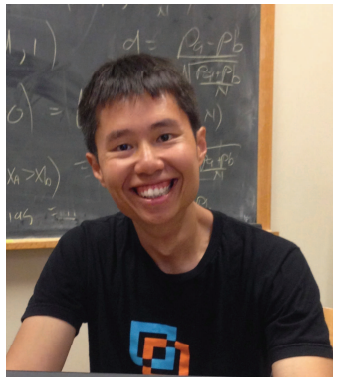
$$|\beta_1| + \sqrt{\theta_1^2 + \theta_2^2}$$

The coefficient of X_1 is nonzero if either group is nonzero; allows one to enforce hierarchy.

We look at two applications:

- Modeling interactions with strong hierarchy — interactions present only when main-effects are present. Project with just-graduated Ph.D student Michael Lim.
- Sparse additive models (SPAM, Ravikumar et al 2009). We use overlap group lasso in a different approach to SPAM models. Work near completion with Ph.D student Alexandra Chouldechova.

Glinternet



Project with PhD student Michael Lim.
Linear + first-order interaction models
using group lasso

Example: GWAS with $p = 27K$ Snps , each a 3-level factor, and a binary response, $N = 3500$.

- Let X_j be $N \times 3$ indicator matrix for each Snp, and $X_{j:k} = X_j \star X_k$ be the $N \times 9$ *interaction* matrix.
- We fit model

$$\log \frac{\Pr(Y = 1|X)}{\Pr(Y = 0|X)} = \alpha + \sum_{j=1}^{p} X_j \beta_j + \sum_{j<k} X_{j:k} \theta_{j:k}$$

- note: $X_{j:k}$ encodes main effects and interactions.

- Maximize group-lasso penalized likelihood:

$$\ell(\mathbf{y}, \mathbf{p}) - \lambda \left[\sum_{j=1}^{p} \|\beta_j\|_2 + \sum_{j<k} \|\theta_{j:k}\|_2 \right]$$

- Solutions map to traditional hierarchical main-effects/interactions model (with effects summing to zero).
- Strong rules essential here — parallel and distributed computing useful too. GWAS search space of 729M interactions!
- GLINTERNET very fast — two-orders of magnitude faster than competition, with similar performance.

Sparse Generalized Additive Models

Work with PhD student Alexandra Chouldechova. Automatic, *sticky* selection between zero, linear or nonlinear terms in GAMs. E.g. $y = \sum_{j=1}^{p} f_j(x_j) + \epsilon$.

$$\frac{1}{2}\left\| y - \sum_{j=1}^{p} \alpha_j x_j - \sum_{j=1}^{p} U_j \beta_j \right\|^2 + \lambda \sum_{j=1}^{p} |\alpha_j| + \gamma\lambda \sum_{j=1}^{p} \sqrt{\mathrm{Tr}\, D^{-1}} \|\beta_j\|_D + \frac{1}{2} \sum_{j=1}^{p} \psi_j \beta_{j2}^T D \beta_{j2}$$

- $U_j = [x_j \; p_1(x_j) \; \cdots \; p_k(x_j)]$ where the p_i are orthogonal Demmler-Reinsch spline basis functions of increasing degree.
- $D = \mathrm{diag}(d_1, \ldots, d_k)$ diagonal penalty matrix with $0 < d_1 \leq d_2 \leq \cdots \leq d_k$

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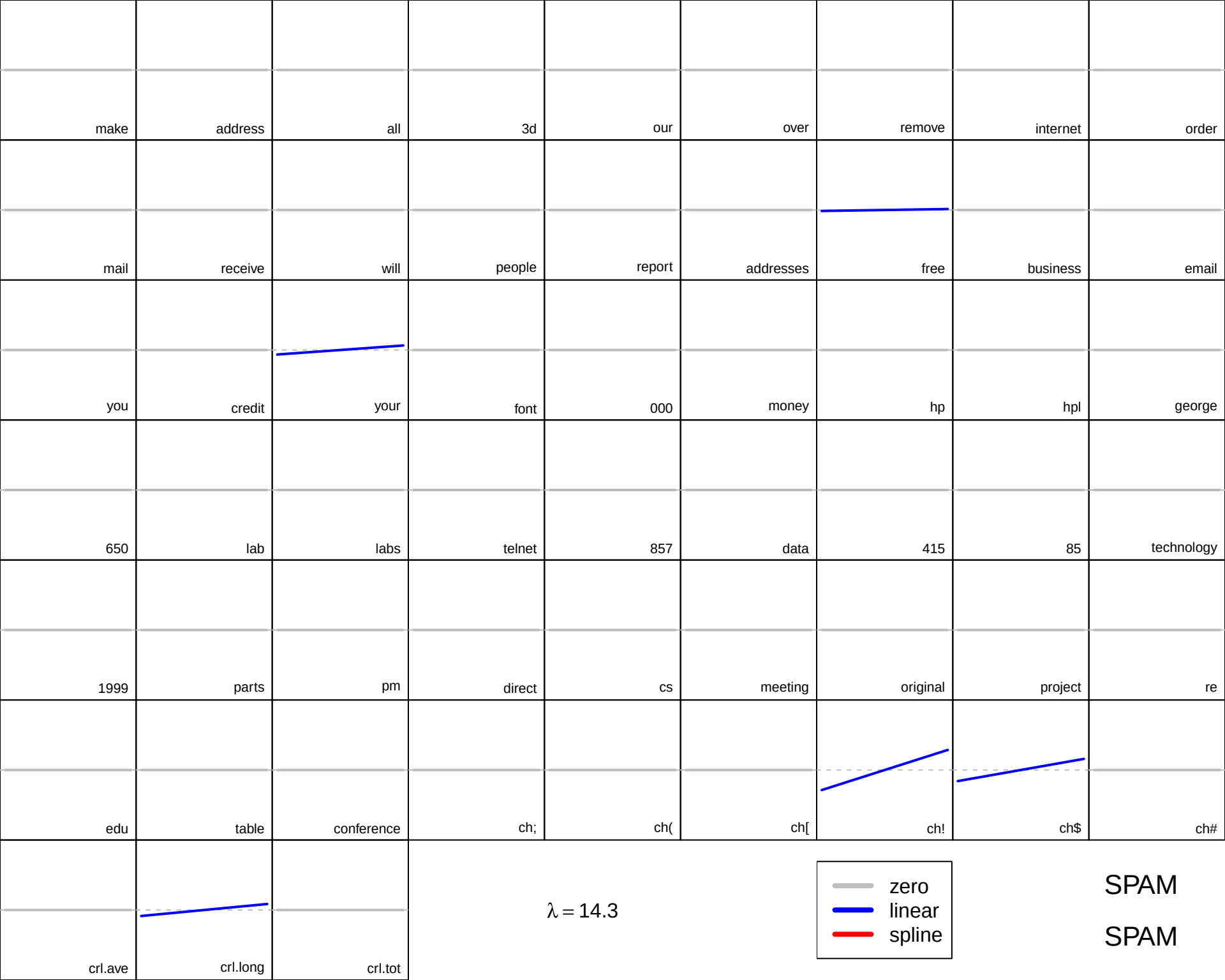
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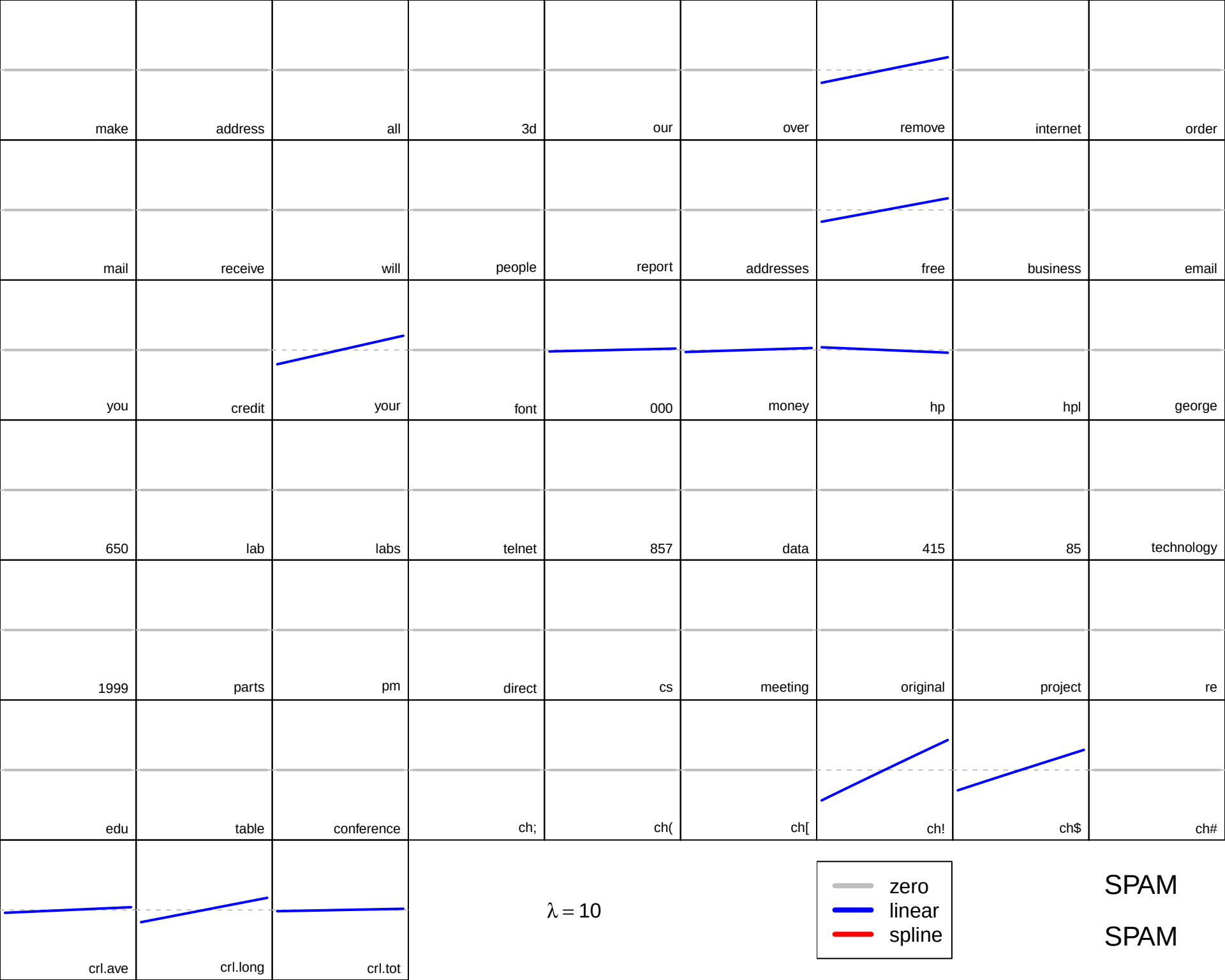
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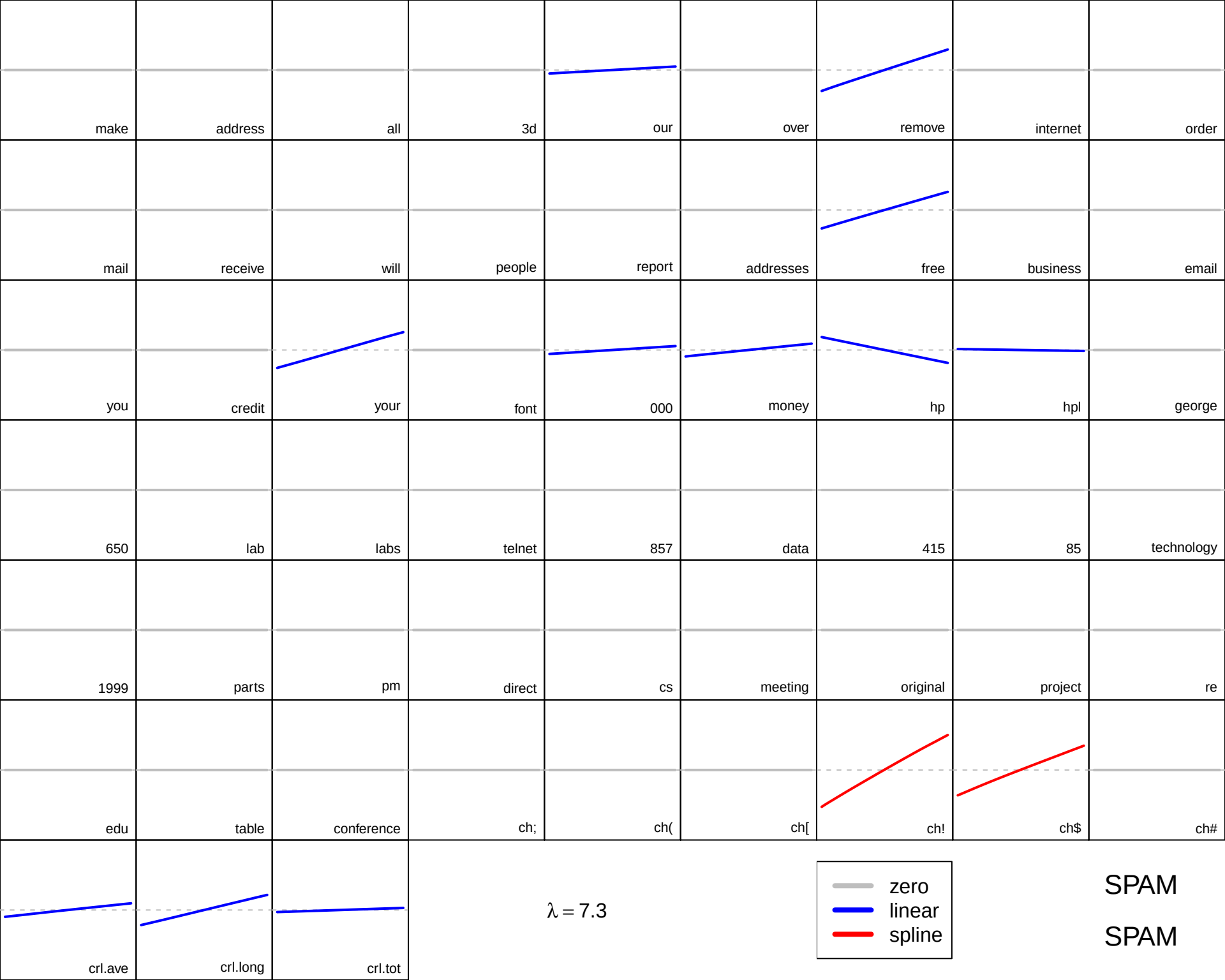
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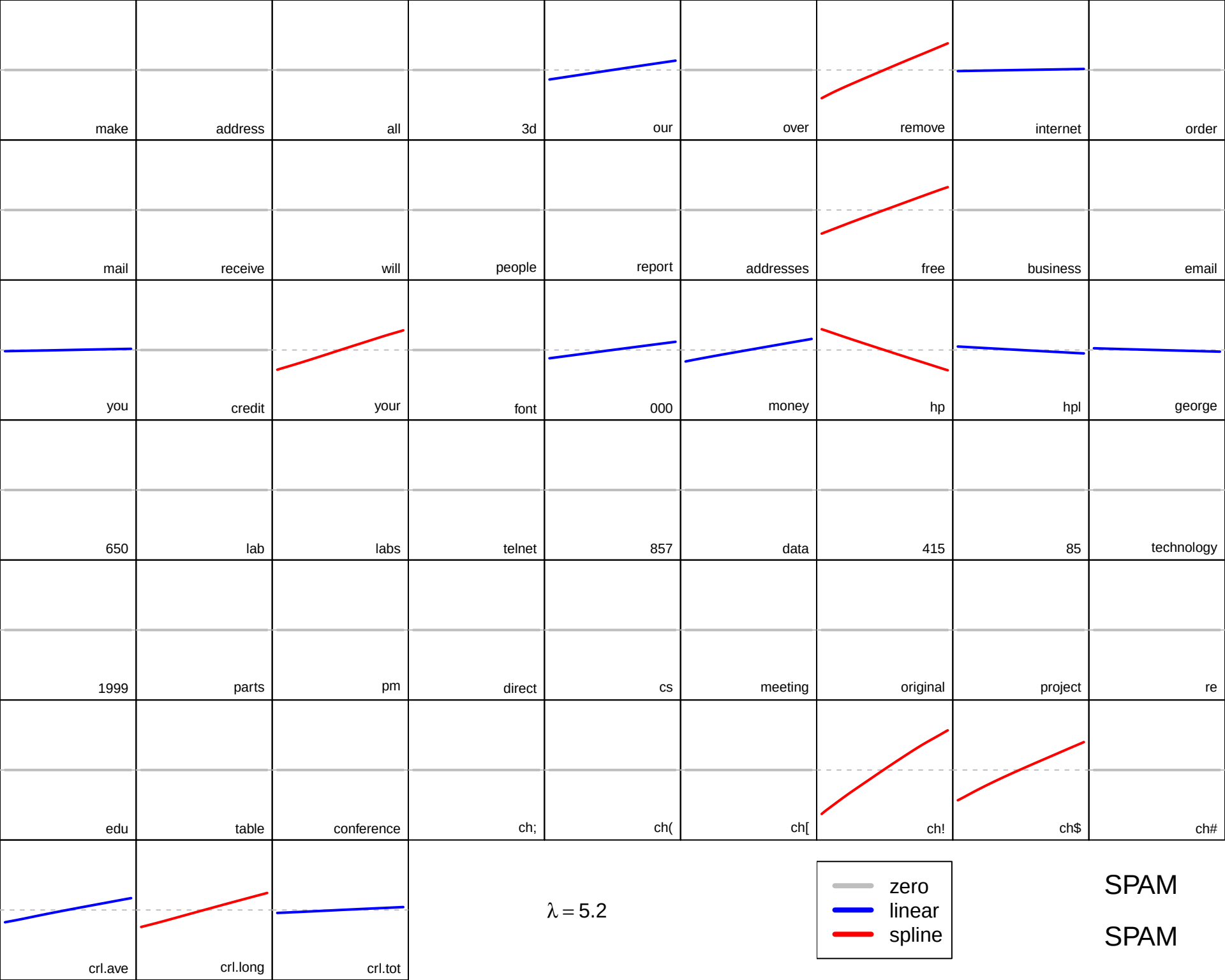
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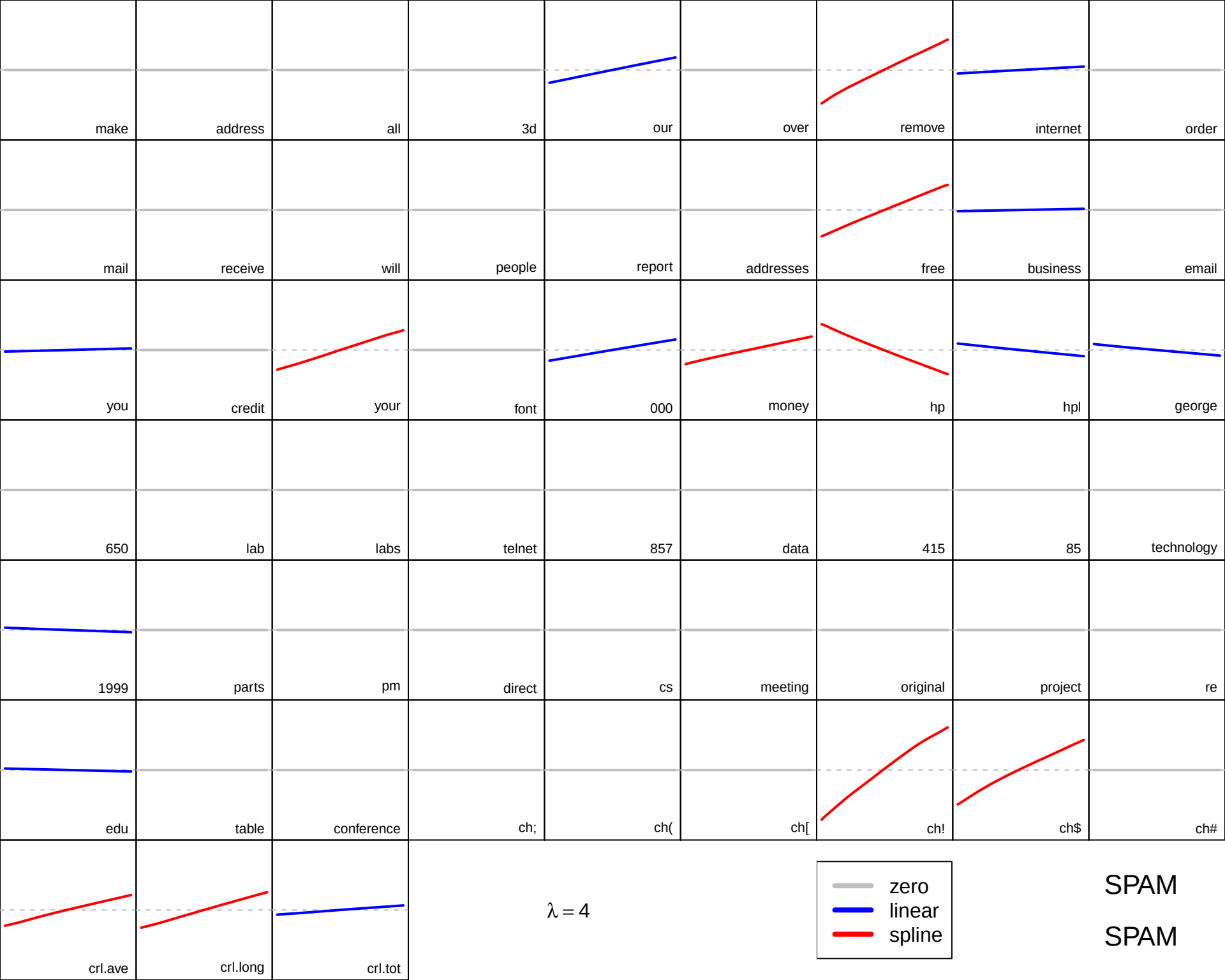
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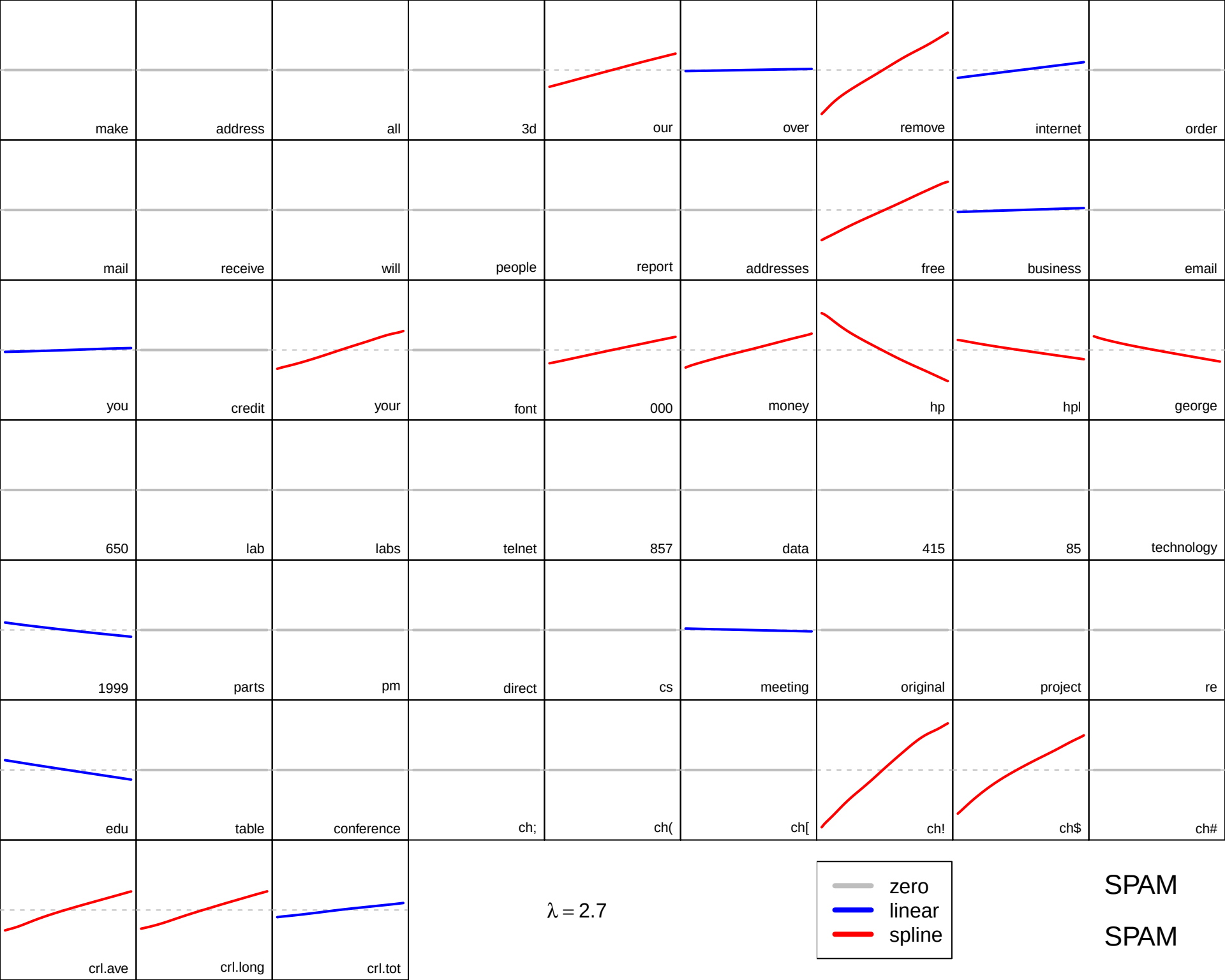
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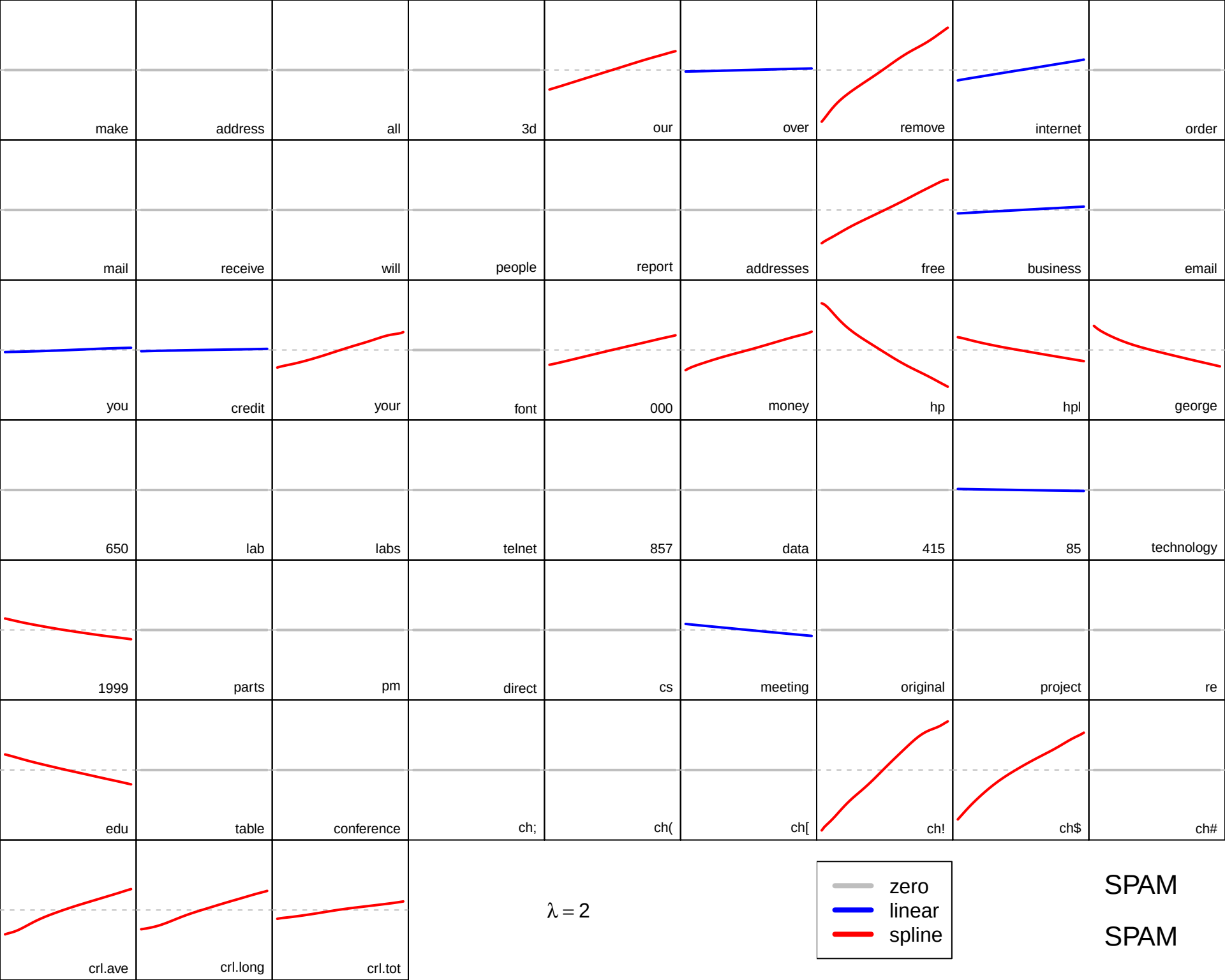
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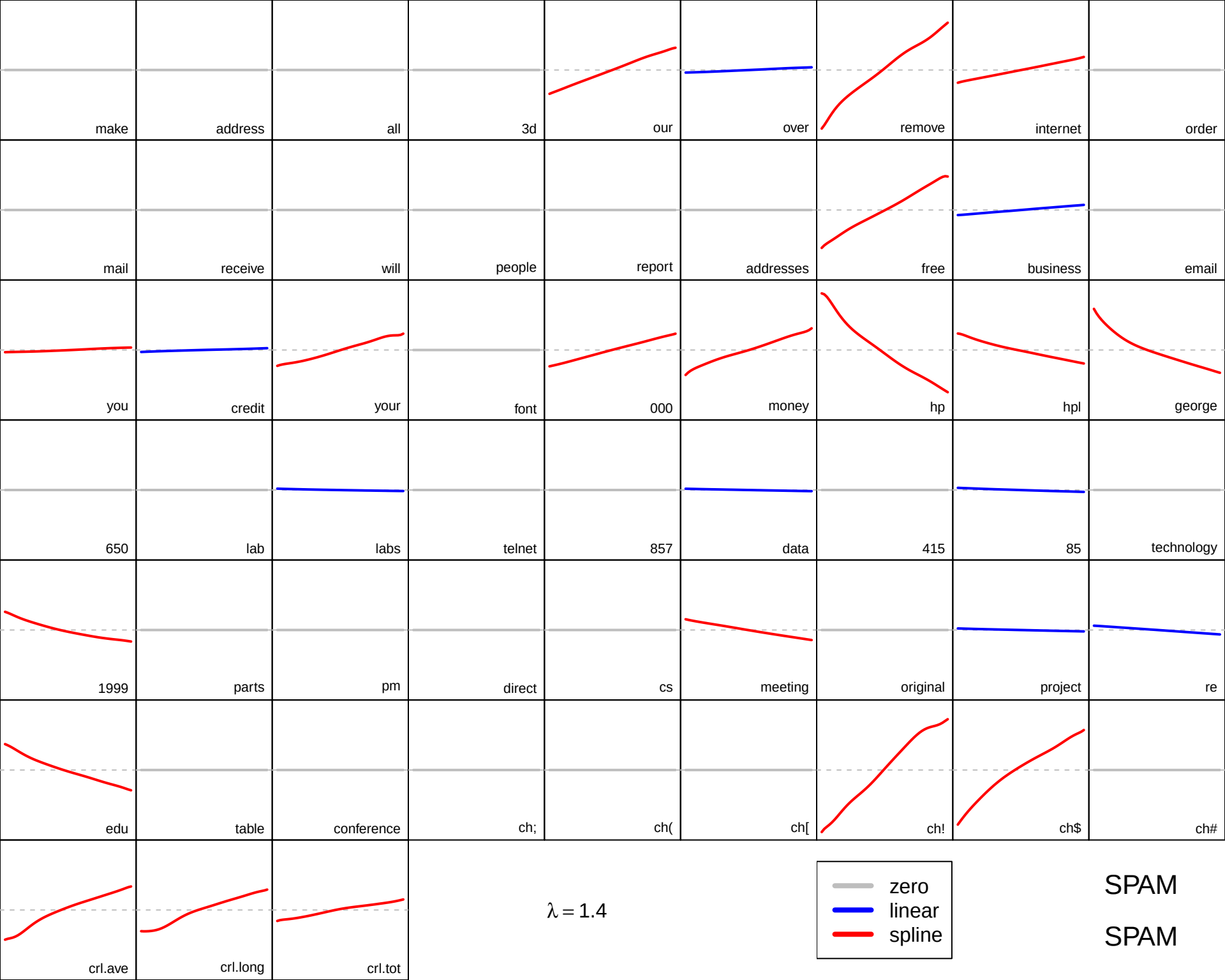
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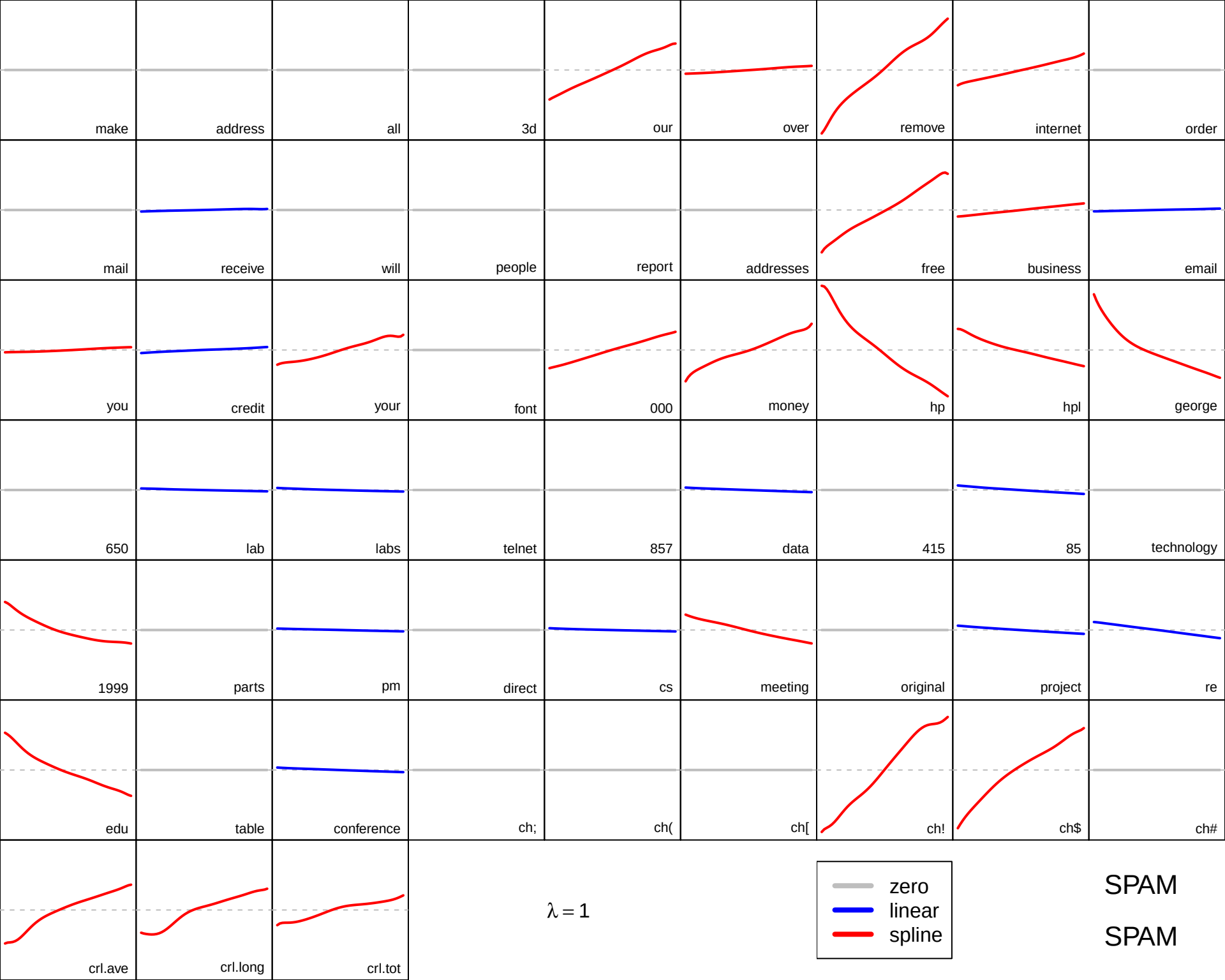
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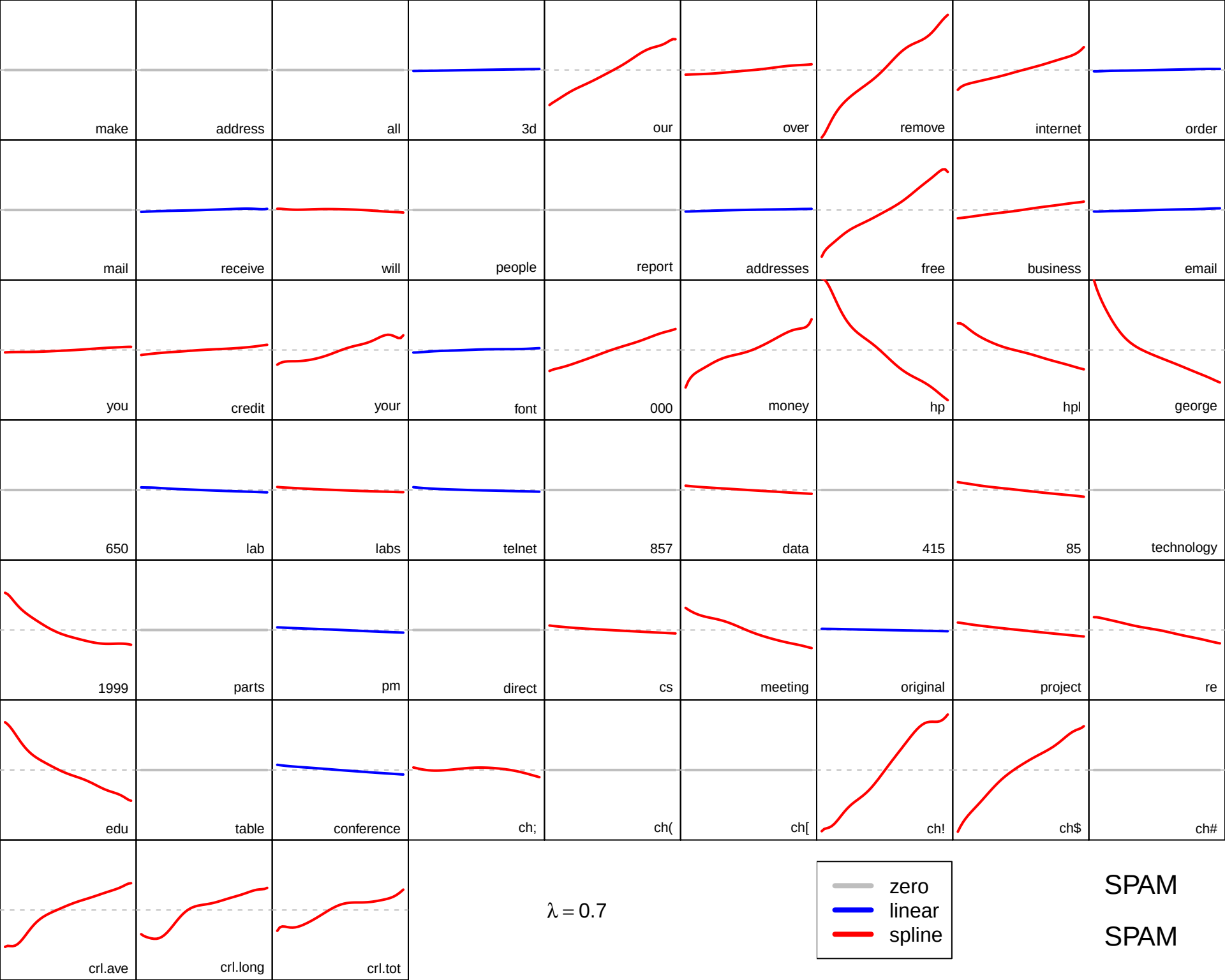
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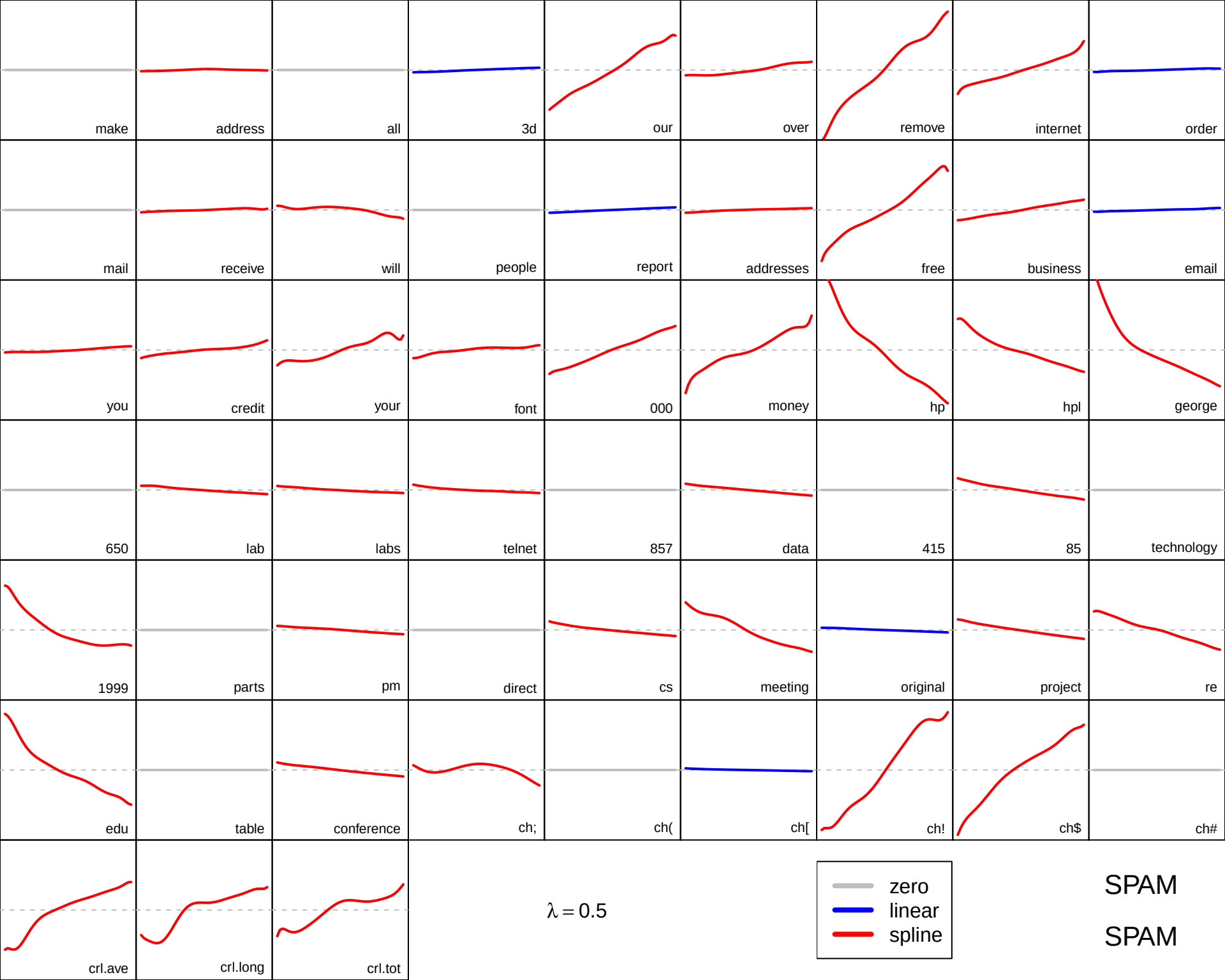
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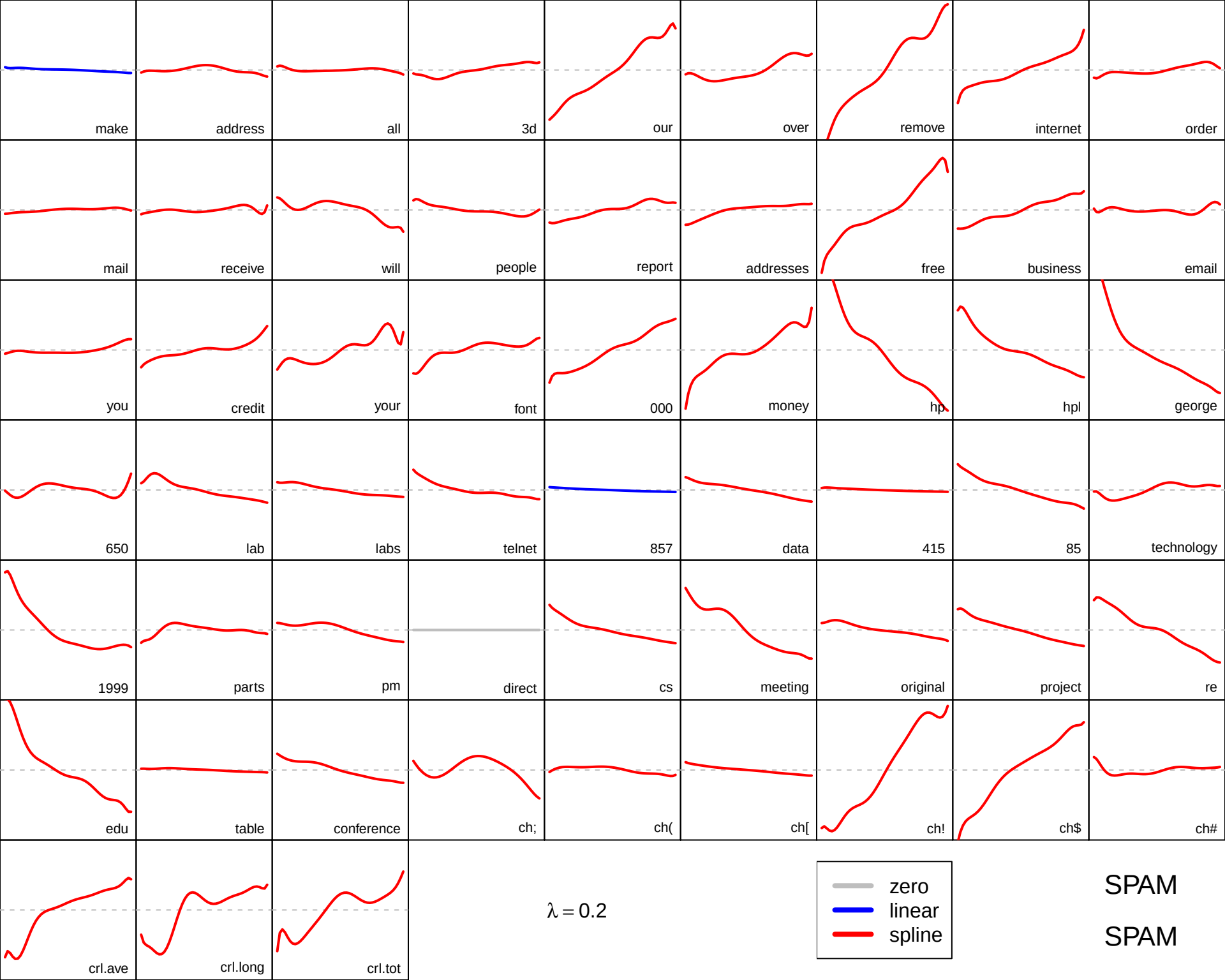
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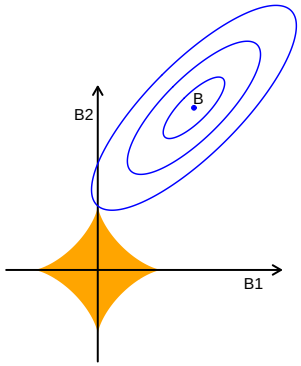
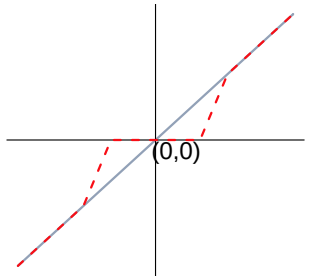
Sparser than Lasso — Concave Penalties

Work with past PhD student Rahul Mazumder and Jerry Friedman (2010).

Extends elastic net family into concave domain

Many approaches. We propose family that bridges ℓ_1 and ℓ_0 based on MC+ penalty (Zhang 2010), and a coordinate-descent scheme for fitting model paths, implemented in SPARSENET



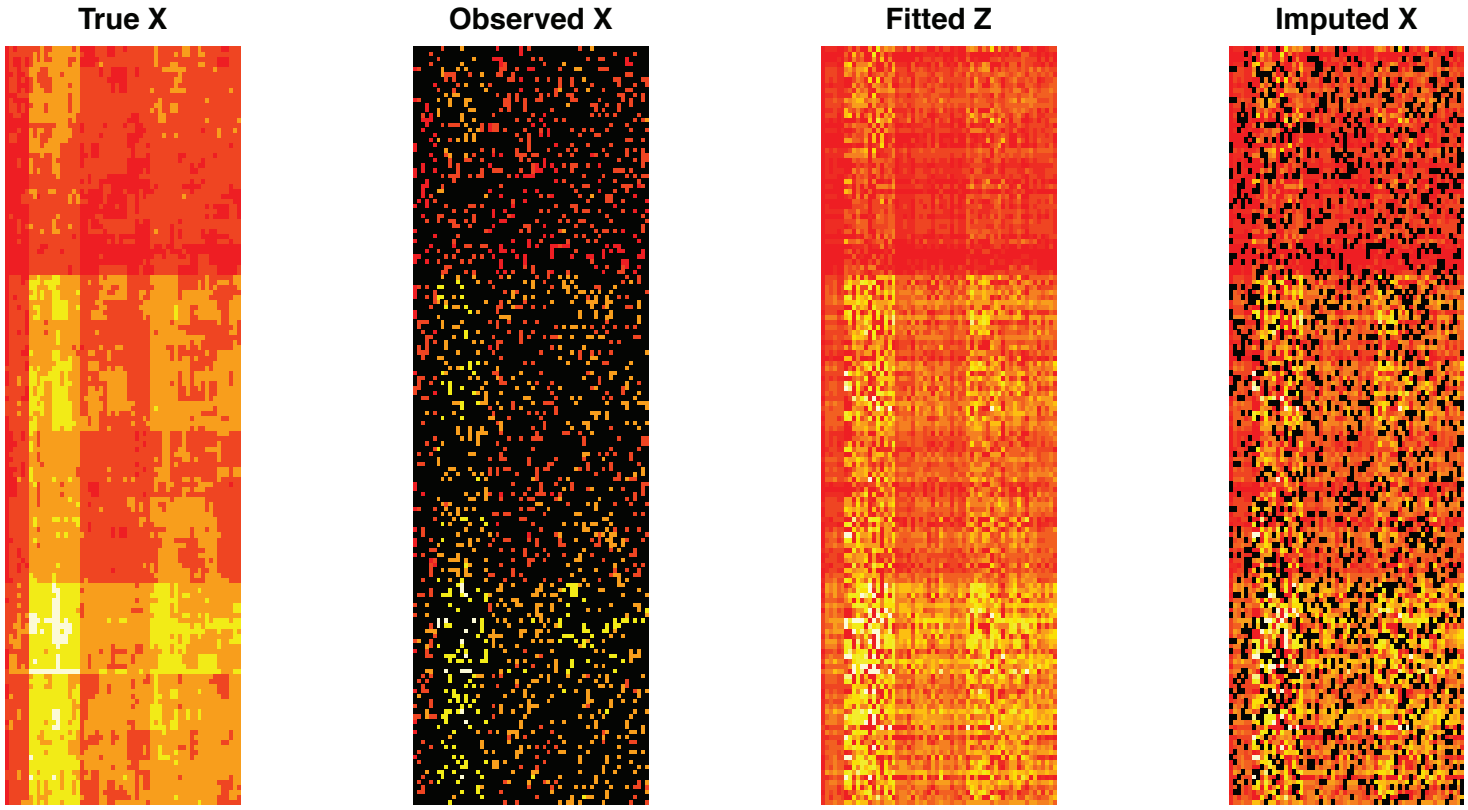


Matrix Completion

- Observe matrix X with (many) missing entries.
- Inspired by SVD, we would like to find $Z_{n\times m}$ of (small) rank r such that training error is small.

$$\min_{Z} \sum_{\text{Observed}(i,j)} (X_{ij} - Z_{ij})^2 \quad \text{subject to } \text{rank}(Z) \leq r$$

- We would then impute the missing X_{ij} with Z_{ij}
- Only problem — this is a nonconvex optimization problem, and unlike SVD for complete X, no closed-form solution.


True X
Observed X
Fitted Z
Imputed X

Nuclear norm and SoftImpute

Use convex relaxation of rank (Candes and Recht, 2008, Mazumder, Hastie and Tibshirani, 2010)

$$\min_{Z} \sum_{\text{Observed}(i,j)} (X_{ij} - Z_{ij})^2 + \lambda ||Z||_*$$

where *nuclear norm* $||Z||_*$ is the sum of singular values of Z.

- Nuclear norm is like the lasso penalty for matrices.
- Solution involves iterative soft-thresholded SVDs of current completed matrix.

Thank You!