Apresentação Final
Diabetes – PIMA

Aprendizagem Estatística em Altas Dimensões
(MAE5904-MAE0501-IBI5904)

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Agenda

Objetivo e Desafios

Objetivo

Prever se a pessoa possui ou não diabetes *mellitus*, com base em uma série de variáveis preditoras.

Desafio

Classificação em banco de dados com muitos dados faltantes.

Banco de Dados PIMA: Variáveis

Variáveis

Variável	Explicação
`Diabetes`	Variável resposta categórica (1 se diabético, 0 se não diabético)
`Pregnancies`	Quantidade de gestações
`Glucose`	Concentração de glicose no plasma após 2 horas em um teste oral de tolerância a glicose
`BloodPressure`	Pressão arterial diastólica (mm Hg)
`SkinThickness`	Espessura da dobra da pele do tríceps (mm)
`Insulin`	Insulina sérica de 2-horas (mu U/ml)
`BMI`	Índice de massa corporal (peso em kg/(altura em m)^2)
`DiabetesPedigreeFunction`	Função "pedigree" de diabetes
`Age`	Idade (anos)

Conjuntos de Treinamento e de Teste

Partição 1: Imputação dos Dados

Total de 768 Observações (100%)

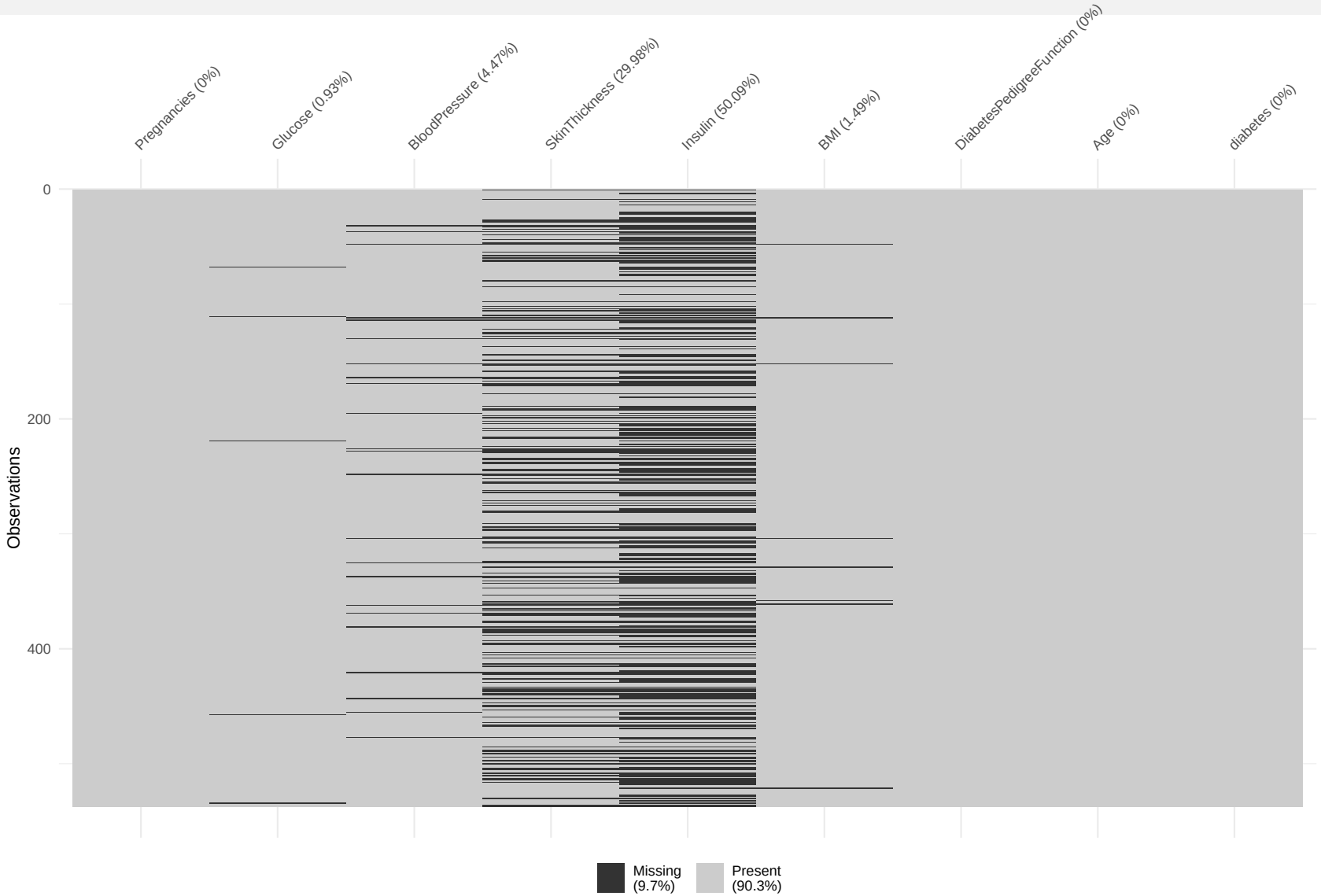
- Treinamento: 537 (70%)
- Teste: 231 (30%)
  - Teste: 161 (70% do Teste)
  - *Out-of-sample*: 70 (30% do Teste)

Partição 2: Eliminação de *Missings*

Total de 382 Observações (100%)

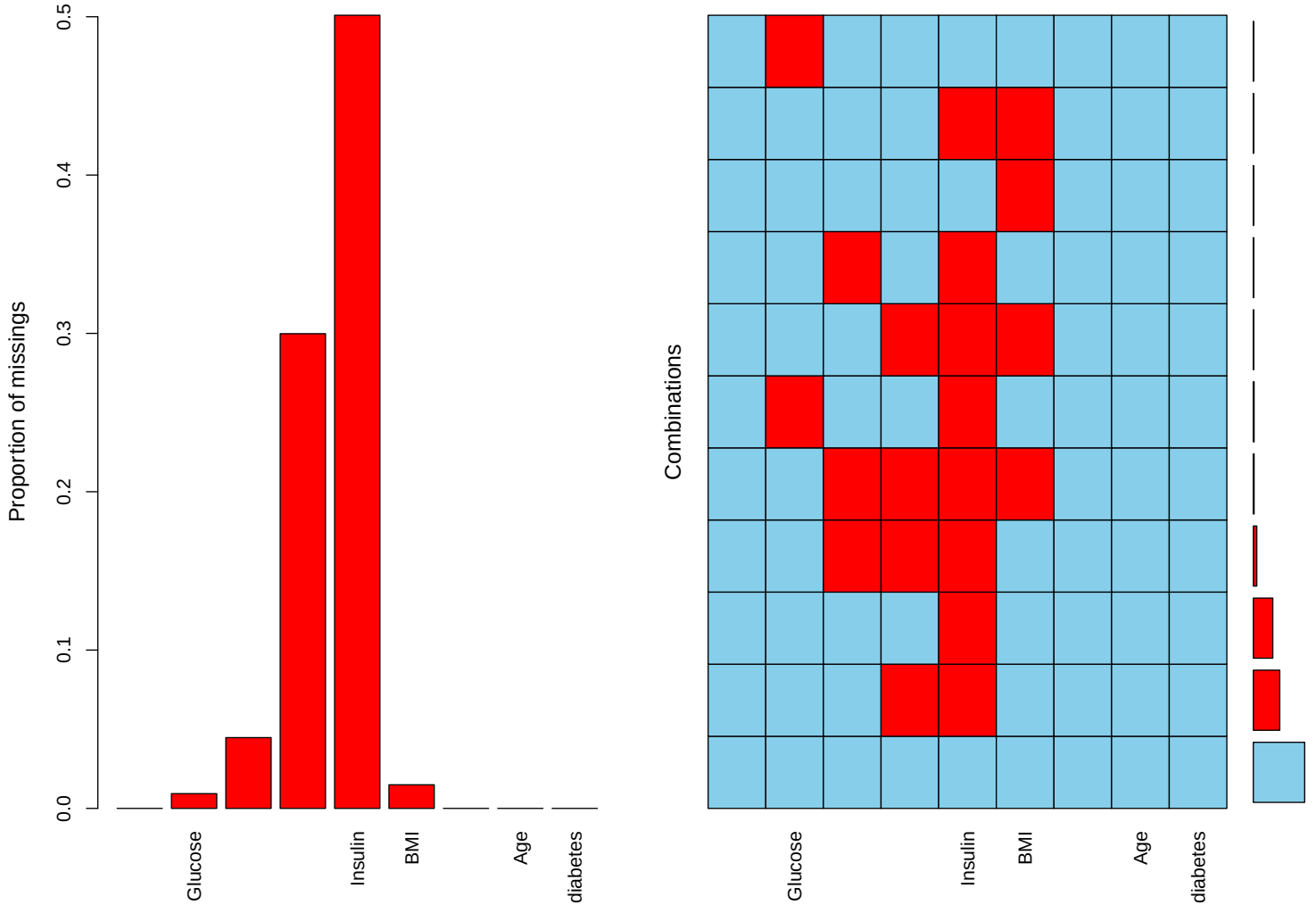
- Treinamento: 266 (70%)
- Teste: 116 (30%)
  - Teste: 89 (77% do Teste)
  - *Out-of-sample*: 27 (23% do Teste)

Padrões nos *Missings*?



Padrões nos *Missings*?

Figura: Frequência de *Missings* e Plot de Combinações



Variáveis com Mais *Missings*

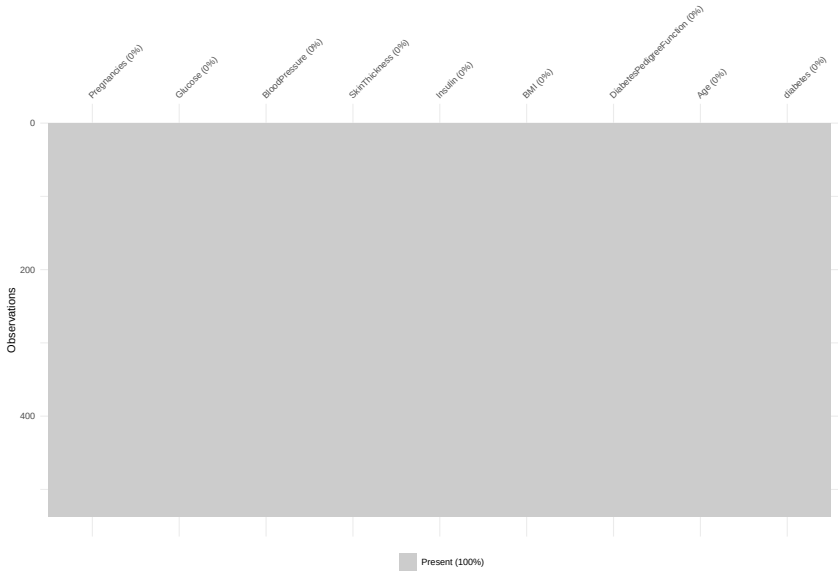
Estratégia de Imputação (Partição 1)

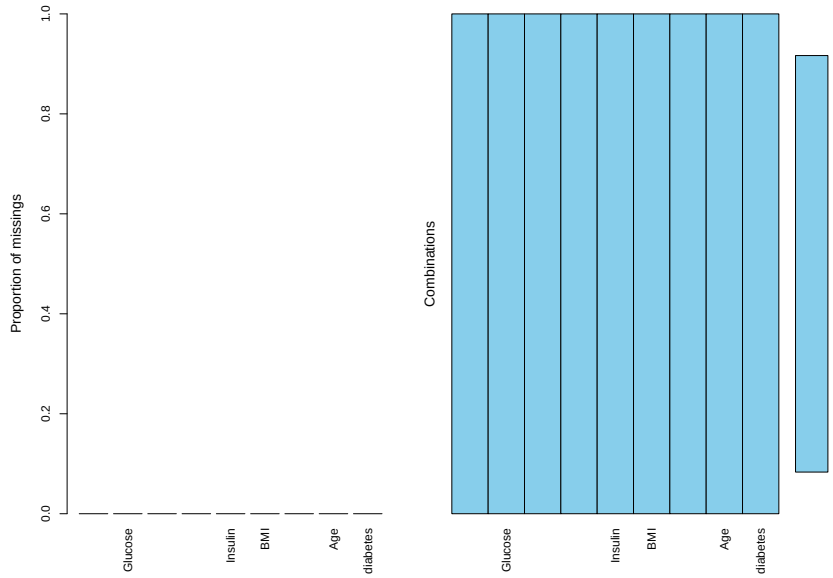
Pacote `mice`

Multivariate Imputation by Chained Equations (MICE)

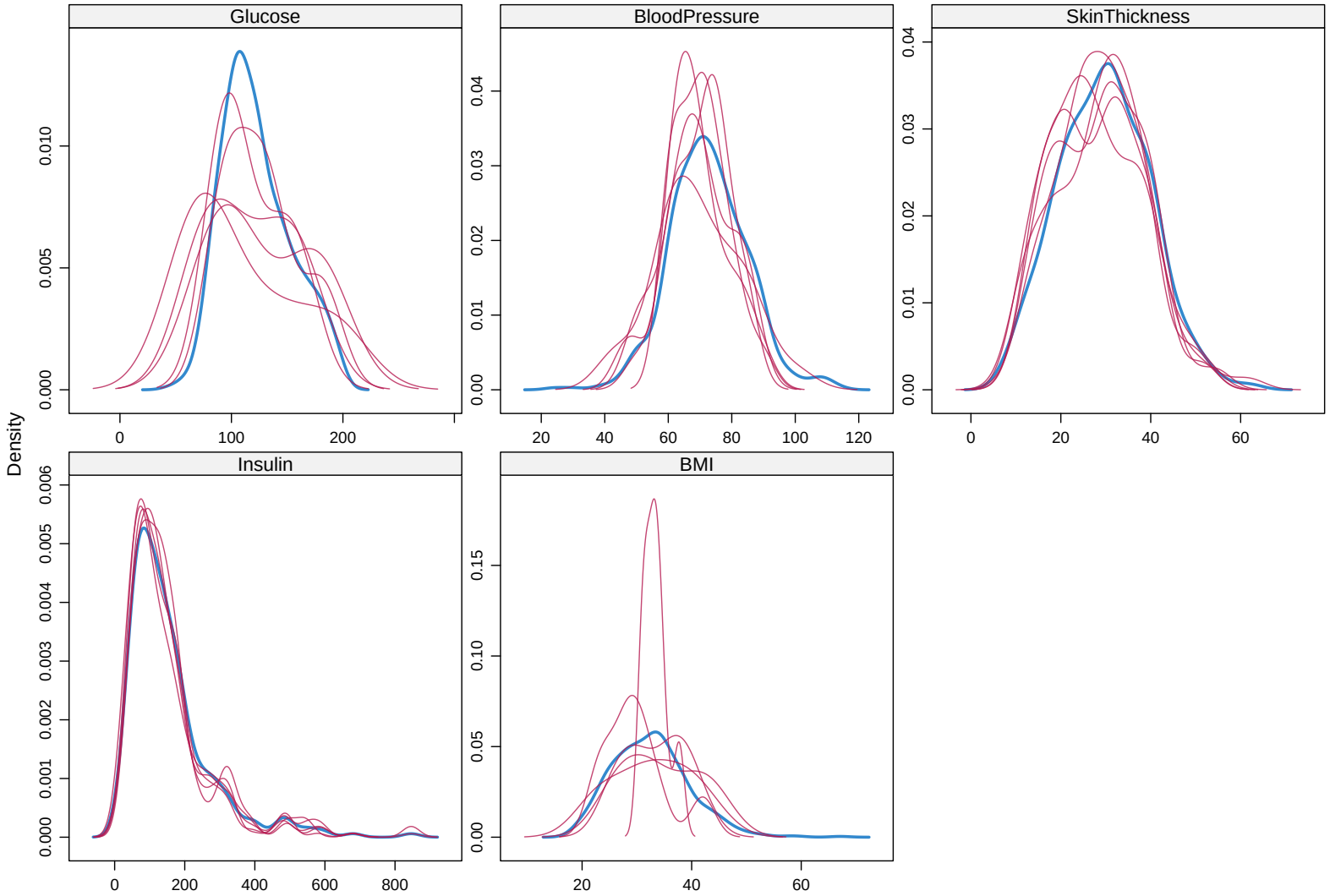
Método `pmm` (*predictive mean matching*)

`https://cran.r-project.org/web/packages/miceRanger/vignettes/miceAlgorithm.html`

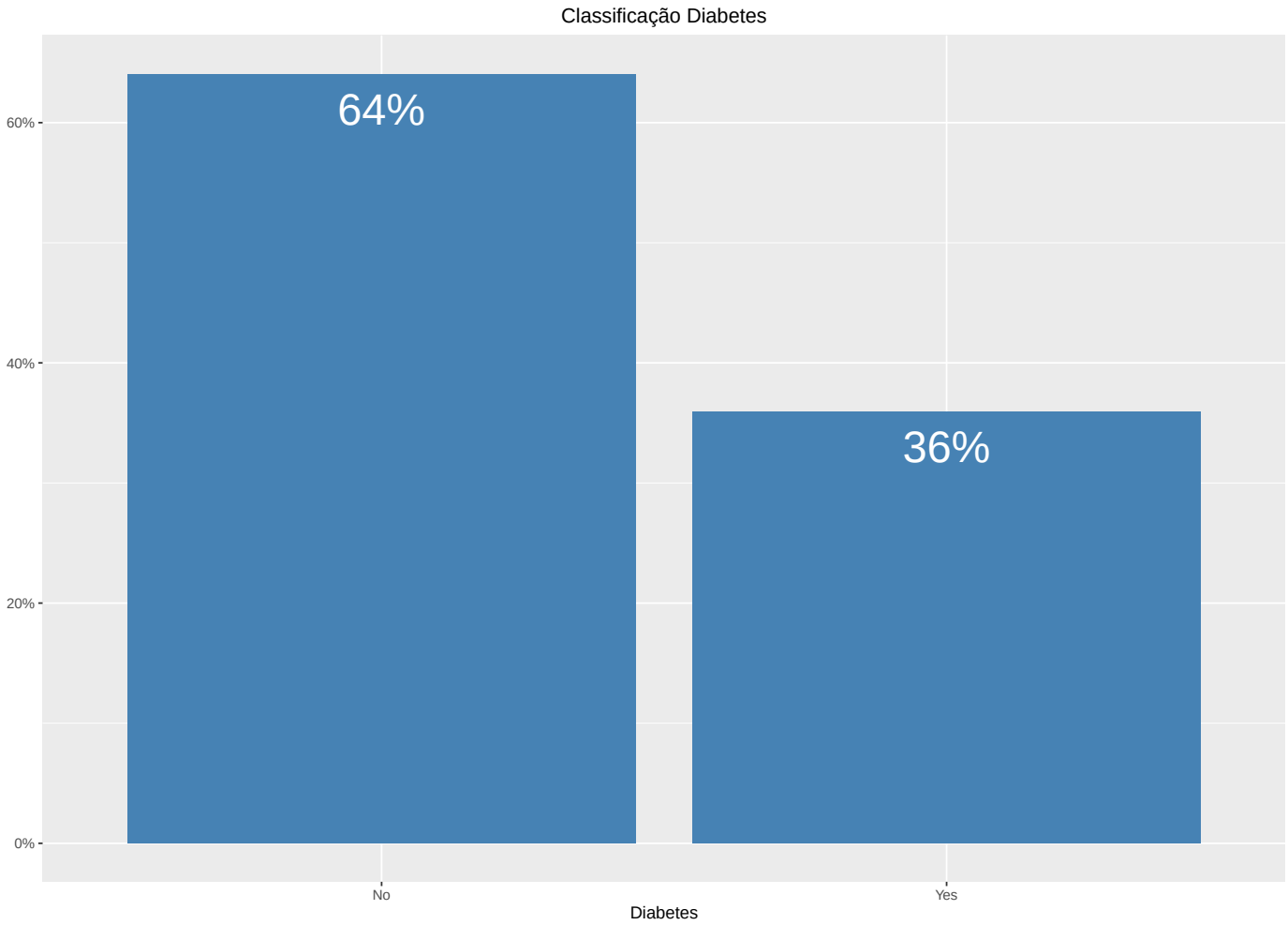


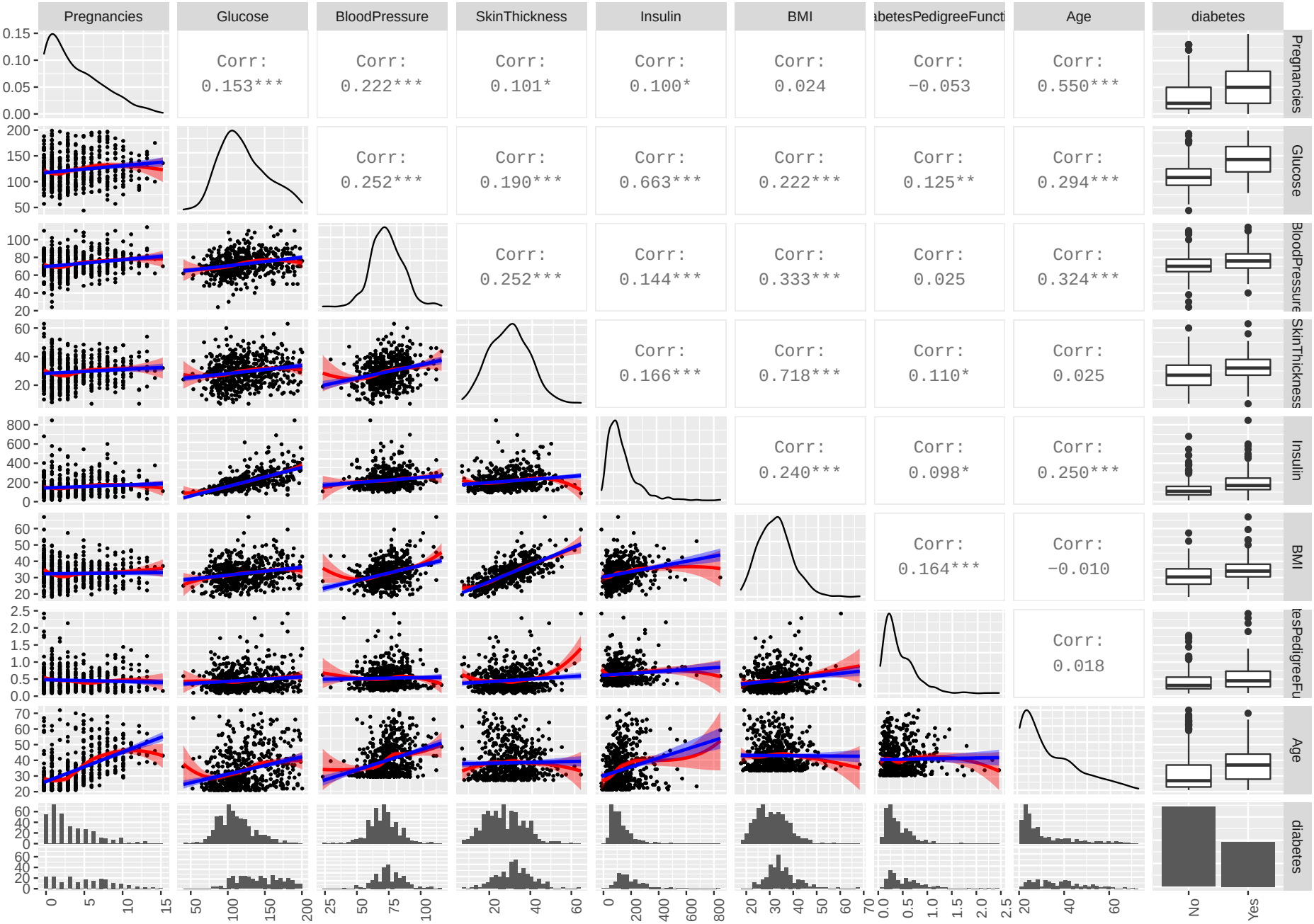


Estratégia de Imputação (Partição 1)

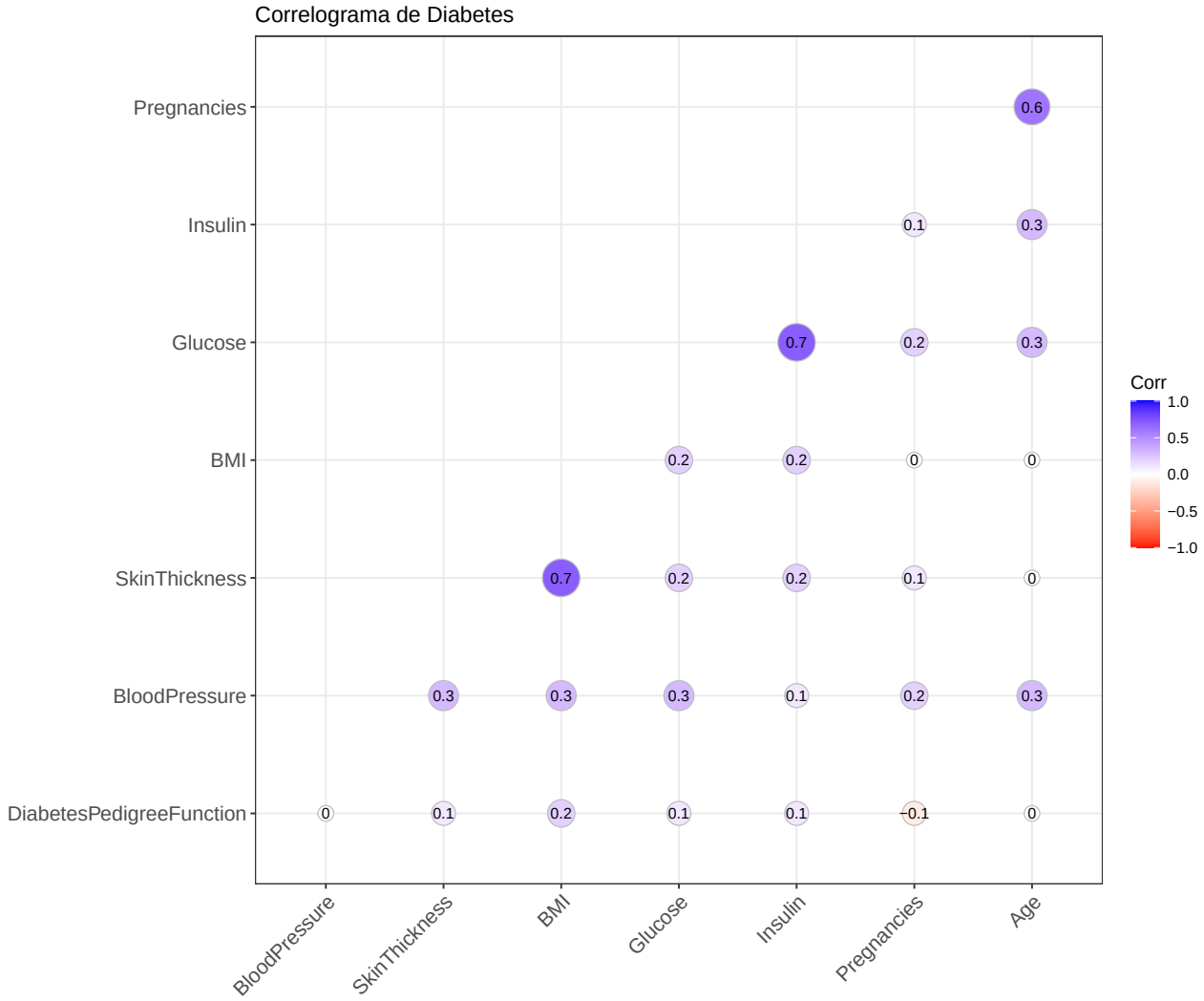


Nos Dados de Treinamento (Sem *Data Snooping*)

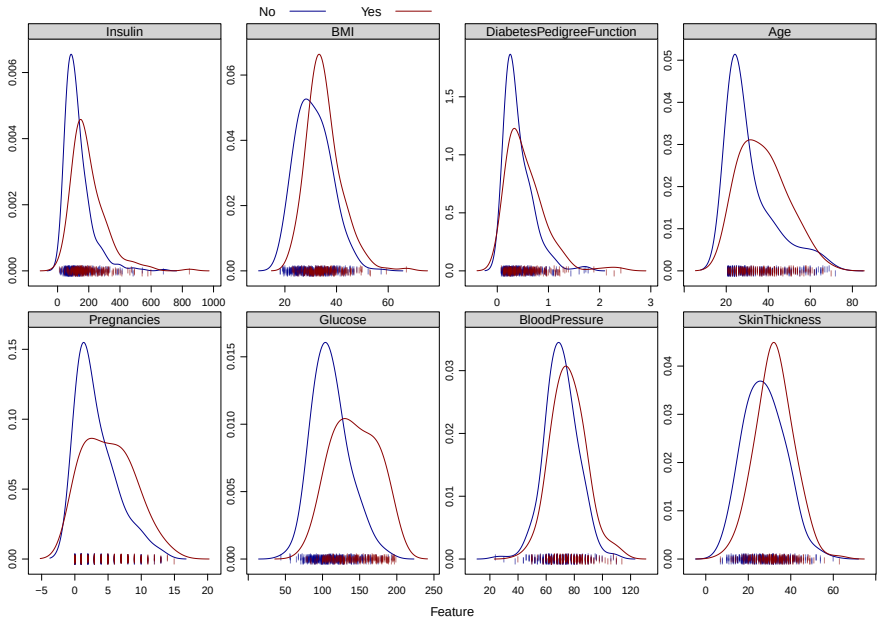


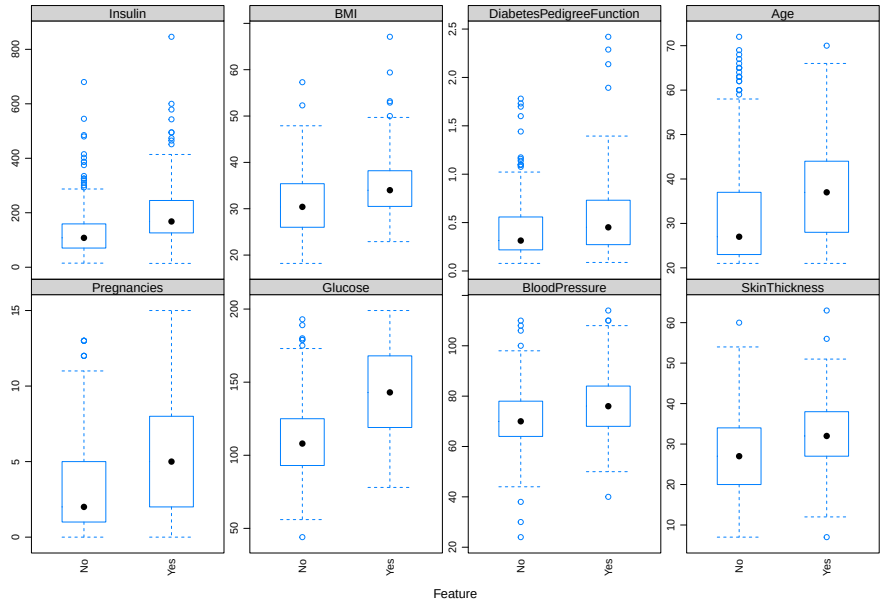

Pregnancies
Glucose
BloodPressure
SkinThickness
Insulin
BMI
abetesPedigreeFunct
Age
diabetes
Corr: 0.153***
Corr: 0.222***
Corr: 0.101*
Corr: 0.100*
Corr: 0.024
Corr: −0.053
Corr: 0.550***
Corr: 0.252***
Corr: 0.190***
Corr: 0.663***
Corr: 0.222***
Corr: 0.125**
Corr: 0.294***
Corr: 0.252***
Corr: 0.144***
Corr: 0.333***
Corr: 0.025
Corr: 0.324***
Corr: 0.166***
Corr: 0.718***
Corr: 0.110*
Corr: 0.025
Corr: 0.240***
Corr: 0.098*
Corr: 0.250***
Corr: 0.164***
Corr: −0.010
Corr: 0.018
No
Yes

Correlograma

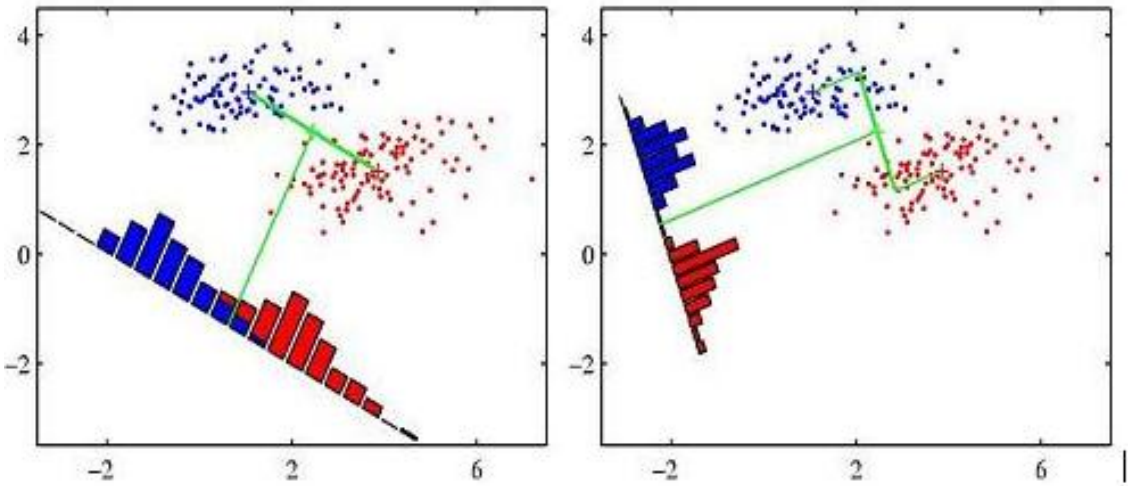


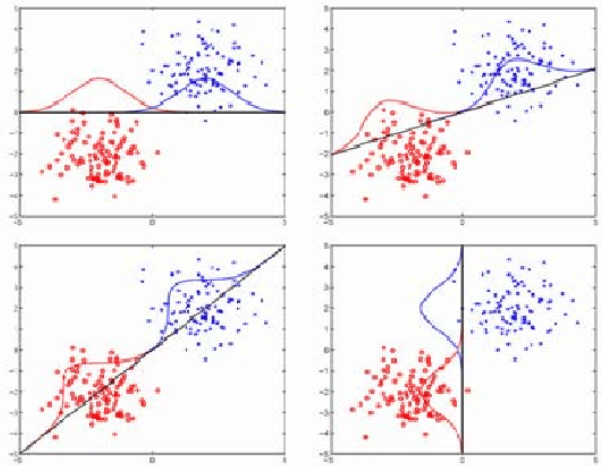
Distribuição por Categoria de Diabetes





Análise Discriminante

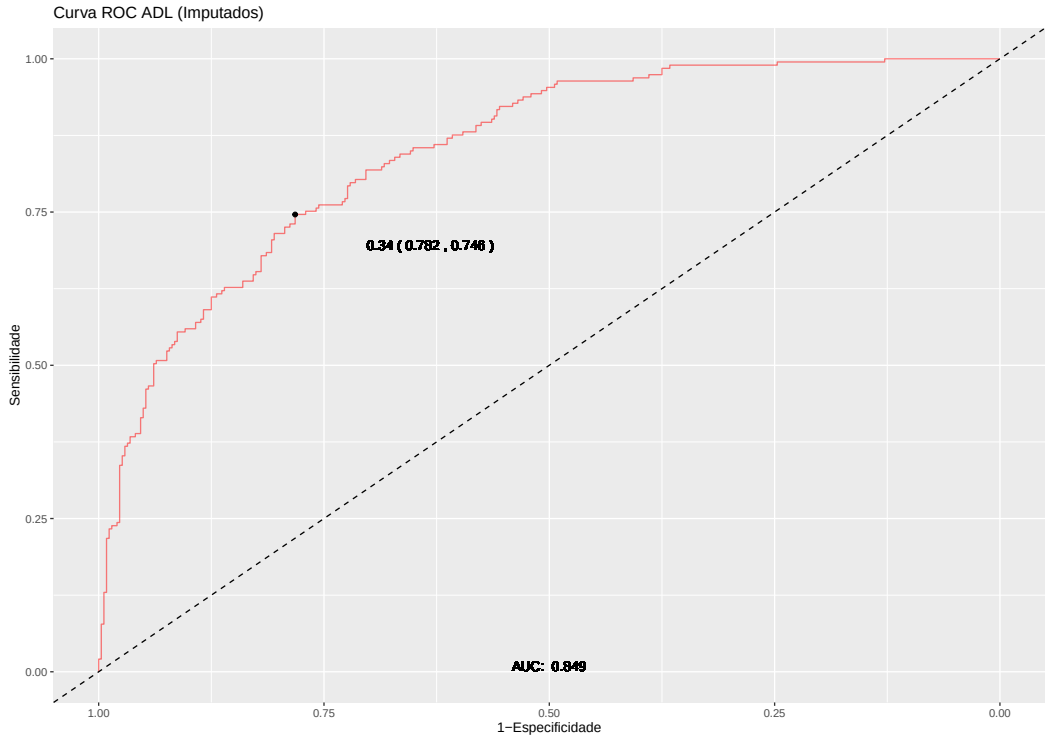




Análise Discriminante Linear (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	99	28
Yes	9	25

- Validação cruzada ($k = 15$)
- Dados imputados

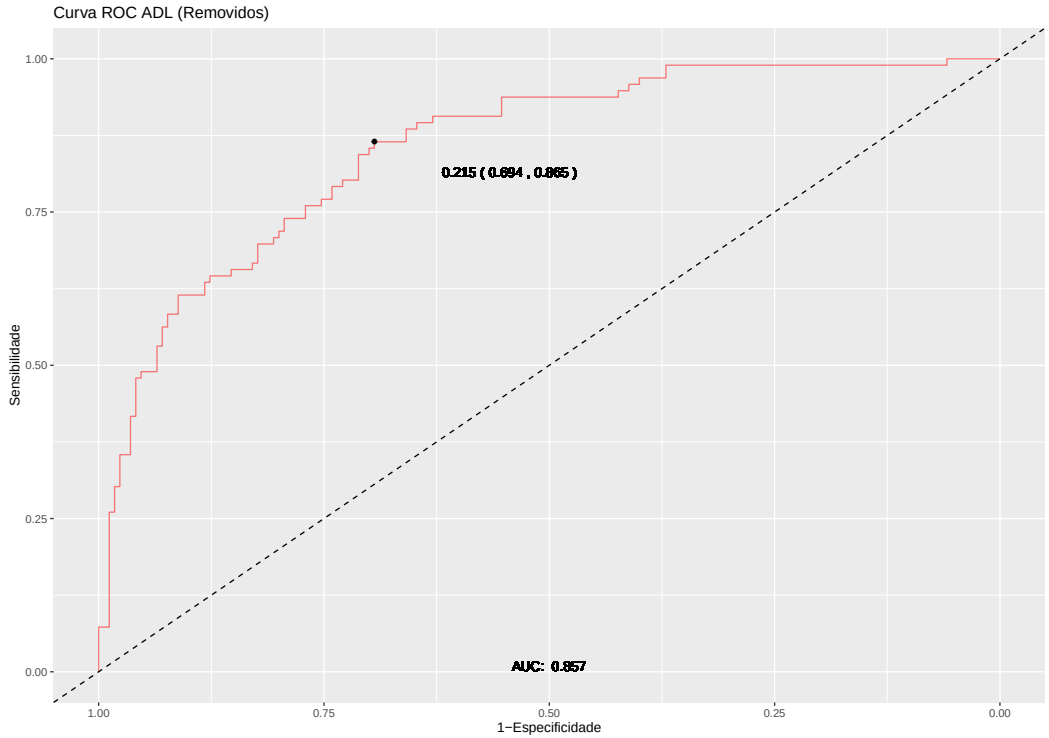


Desempenho do Modelo			
Accuracy	0.7702	**Sensitivity**	0.9167
95% CI	(0.6974, 0.8327)	**Specificity**	0.4717
No Information Rate	0.6708	**Pos Pred Value**	0.7795
P-Value [Acc >NIR]	0.003815	**Neg Pred Value**	0.7353
		Prevalence	0.6708
Kappa	0.4274	**Detection Rate**	0.6149
		Detection Prevalence	0.7888
Mcnemar's Test P-Value	0.003085	**Balanced Accuracy**	0.6942

Análise Discriminante Linear (Partição 2)

	Referência	
Predito	**No**	**Yes**
No	64	12
Yes	4	9

- Validação cruzada ($k = 15$)
- Dados sem *missings*

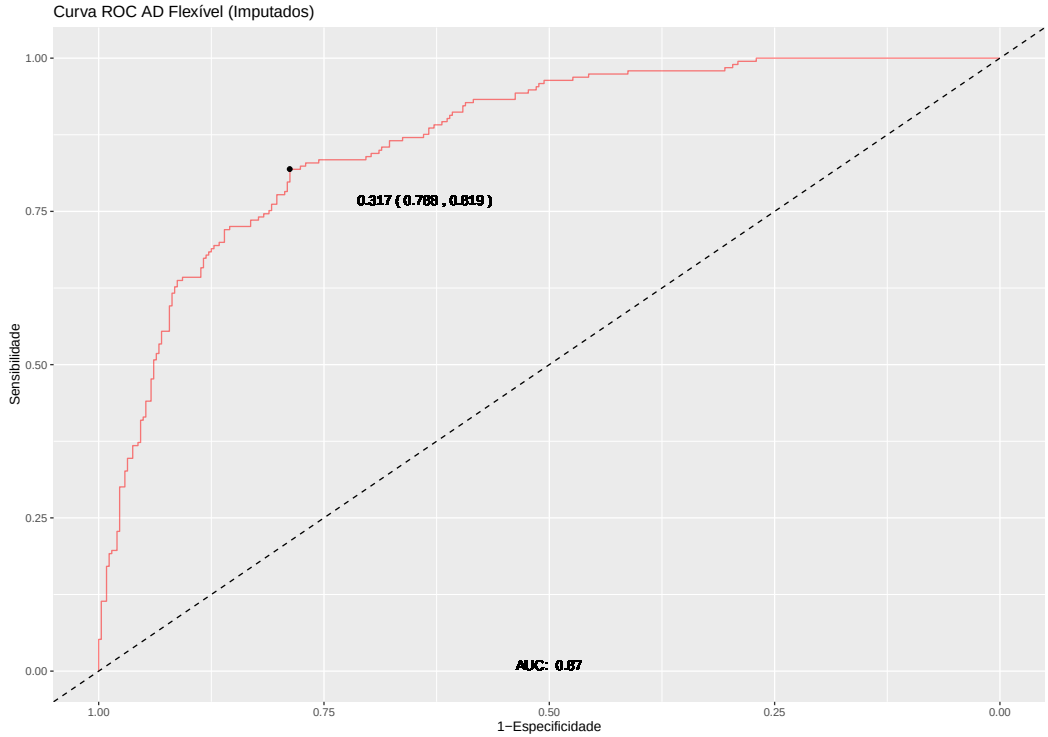


Desempenho do Modelo			
Accuracy	0.8202	**Sensitivity**	0.9412
95% CI	(0.7245, 0.8936)	**Specificity**	0.4286
No Information Rate	0.764	**Pos Pred Value**	0.8421
P-Value [Acc >NIR]	0.12910	**Neg Pred Value**	0.6923
		Prevalence	0.7640
Kappa	0.4258	**Detection Rate**	0.7191
		Detection Prevalence	0.8539
Mcnemar's Test P-Value	0.08012	**Balanced Accuracy**	0.6849

Análise Discriminante Flexível (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	95	25
Yes	13	28

- Validação cruzada ($k = 15$)
- Dados imputados

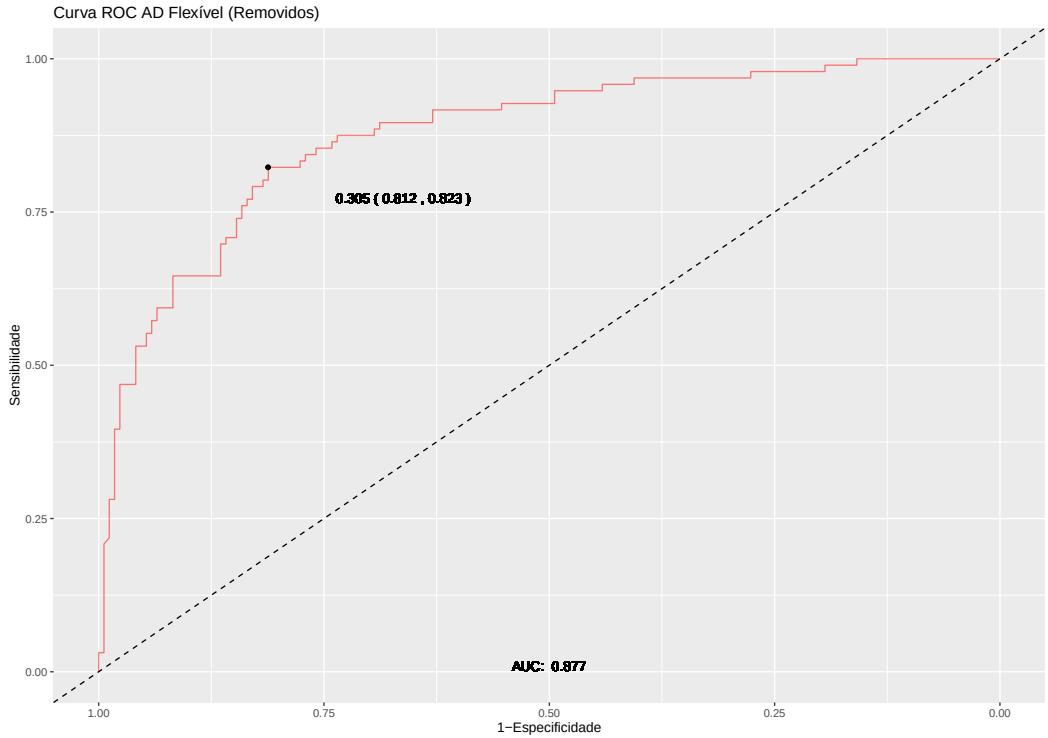


Desempenho do Modelo			
Accuracy	0.764	**Sensitivity**	0.8796
95% CI	(0.6907, 0.8272)	**Specificity**	0.5283
No Information Rate	0.6708	**Pos Pred Value**	0.7917
P-Value [Acc >NIR]	0.006397	**Neg Pred Value**	0.6829
		Prevalence	0.6708
Kappa	0.4329	**Detection Rate**	0.5901
		Detection Prevalence	0.7453
Mcnemar's Test P-Value	0.074353	**Balanced Accuracy**	0.7040

Análise Discriminante Flexível (Partição 2)

	Referência	
Predito	**No**	**Yes**
No	61	11
Yes	7	10

- Validação cruzada ($k = 15$)
- Dados sem *missings*

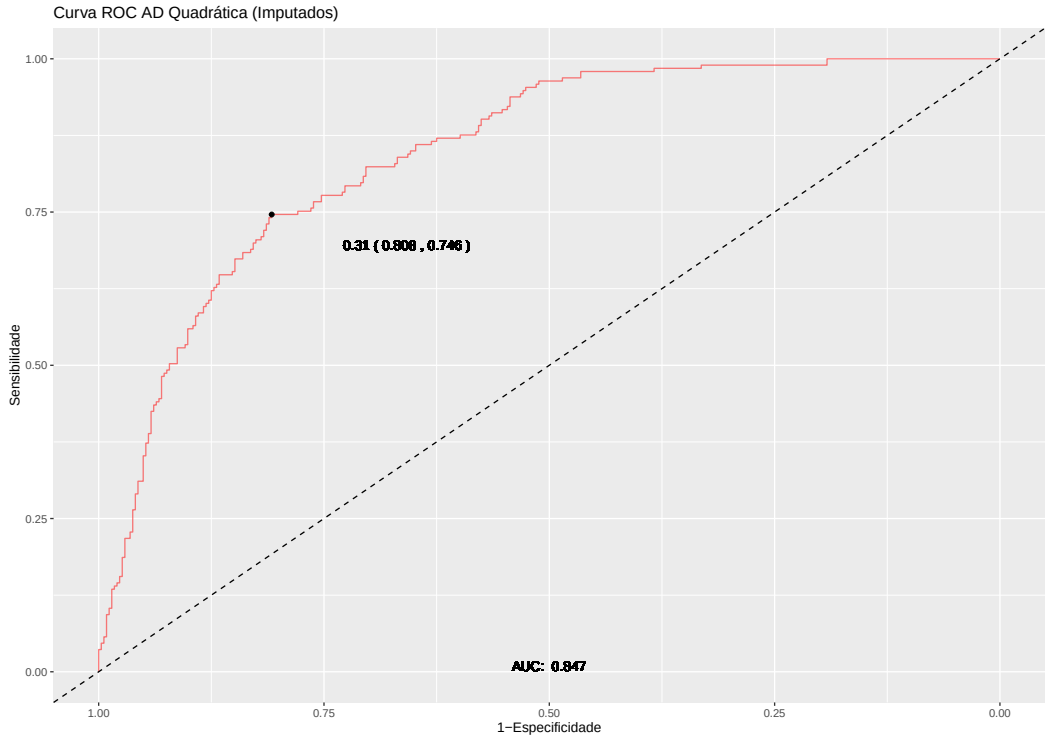


Desempenho do Modelo			
Accuracy	0.7978	**Sensitivity**	0.8971
95% CI	(0.6993, 0.8755)	**Specificity**	0.4762
No Information Rate	0.764	**Pos Pred Value**	0.8472
P-Value [Acc >NIR]	0.2709	**Neg Pred Value**	0.5882
		Prevalence	0.7640
Kappa	0.3996	**Detection Rate**	0.6854
		Detection Prevalence	0.8090
Mcnemar's Test P-Value	0.4795	**Balanced Accuracy**	0.6866

Análise Discriminante Quadrática (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	96	27
Yes	12	26

- Validação cruzada ($k = 15$)
- Dados imputados

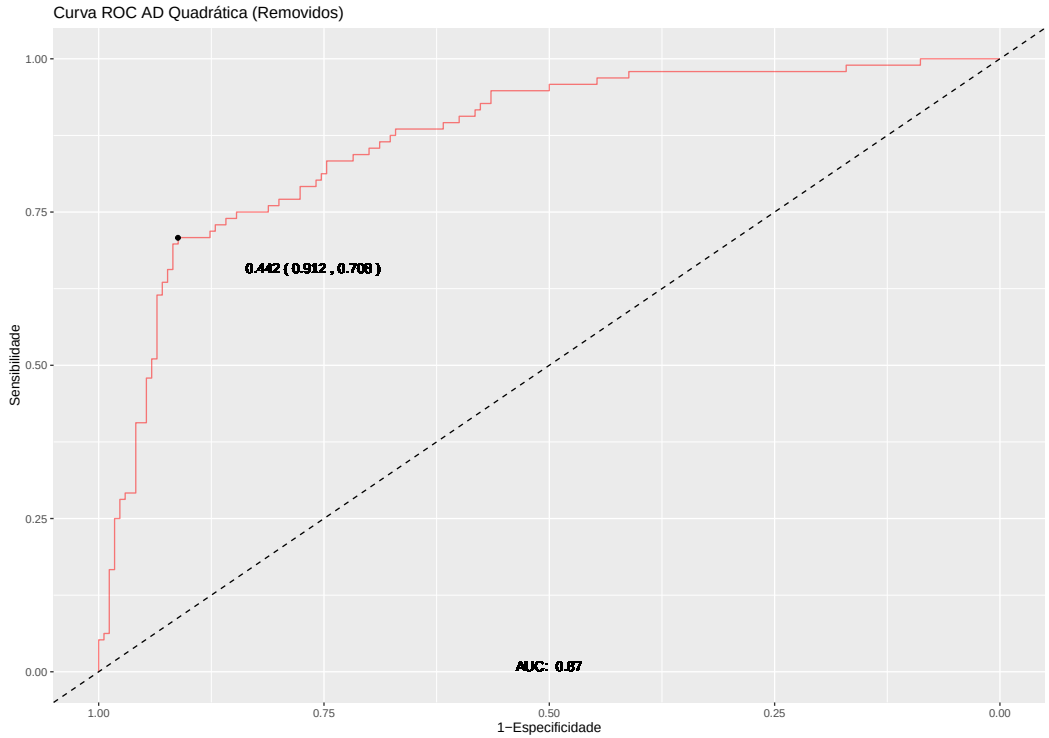


Desempenho do Modelo			
Accuracy	0.7578	**Sensitivity**	0.8889
95% CI	(0.6841, 0.8217)	**Specificity**	0.4906
No Information Rate	0.6708	**Pos Pred Value**	0.7805
P-Value [Acc >NIR]	0.01039	**Neg Pred Value**	0.6842
		Prevalence	0.6708
Kappa	0.4089	**Detection Rate**	0.5963
		Detection Prevalence	0.7640
Mcnemar's Test P-Value	0.02497	**Balanced Accuracy**	0.6897

Análise Discriminante Quadrática (Partição 2)

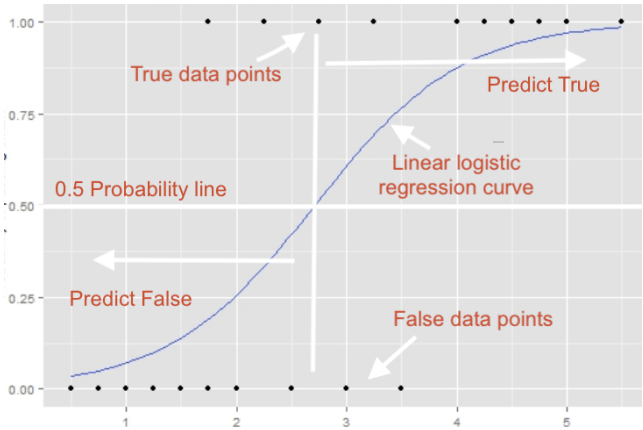
	Referência	
Predito	**No**	**Yes**
No	60	6
Yes	8	15

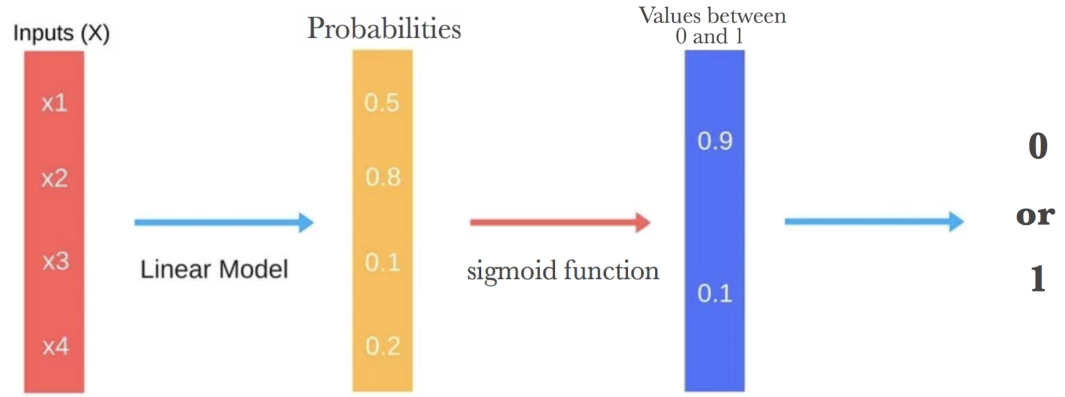
- Validação cruzada ($k = 15$)
- Dados sem *missings*



Desempenho do Modelo			
Accuracy	0.8427	**Sensitivity**	0.8824
95% CI	(0.7502, 0.9112)	**Specificity**	0.7143
No Information Rate	0.764	**Pos Pred Value**	0.9091
P-Value [Acc >NIR]	0.04778	**Neg Pred Value**	0.6522
		Prevalence	0.7640
Kappa	0.5776	**Detection Rate**	0.6742
		Detection Prevalence	0.7416
Mcnemar's Test P-Value	0.78927	**Balanced Accuracy**	0.7983

Regressão Logística

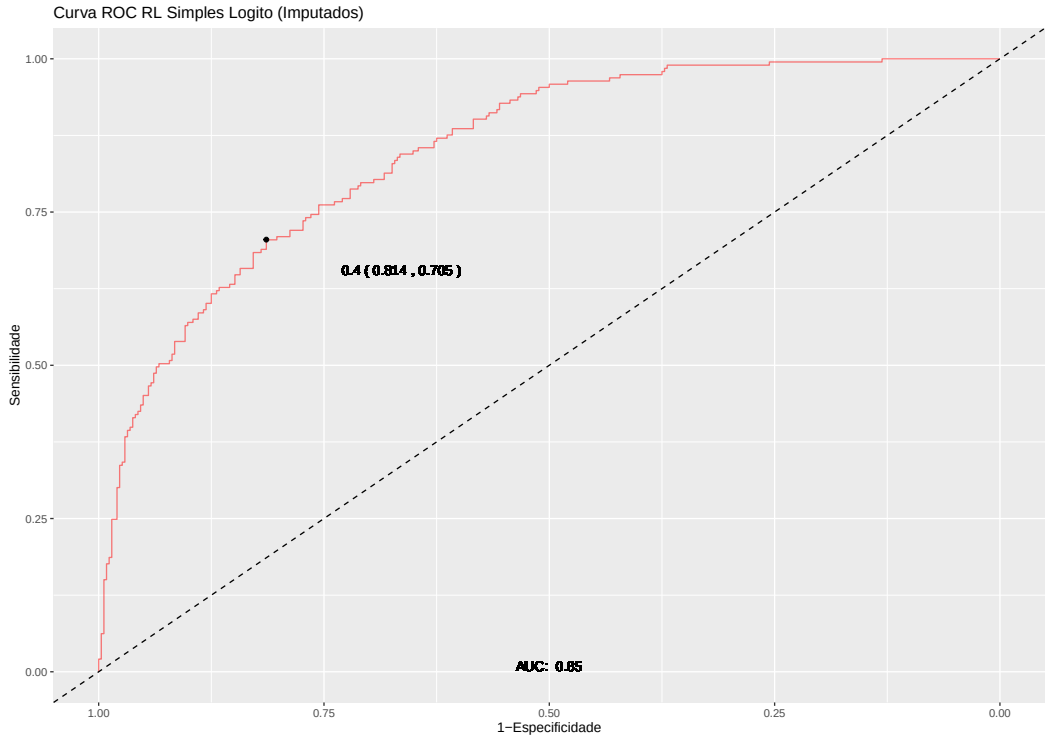




Regressão Logística Simples (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	99	27
Yes	9	26

- Validação cruzada ($k = 10$)
- Dados imputados

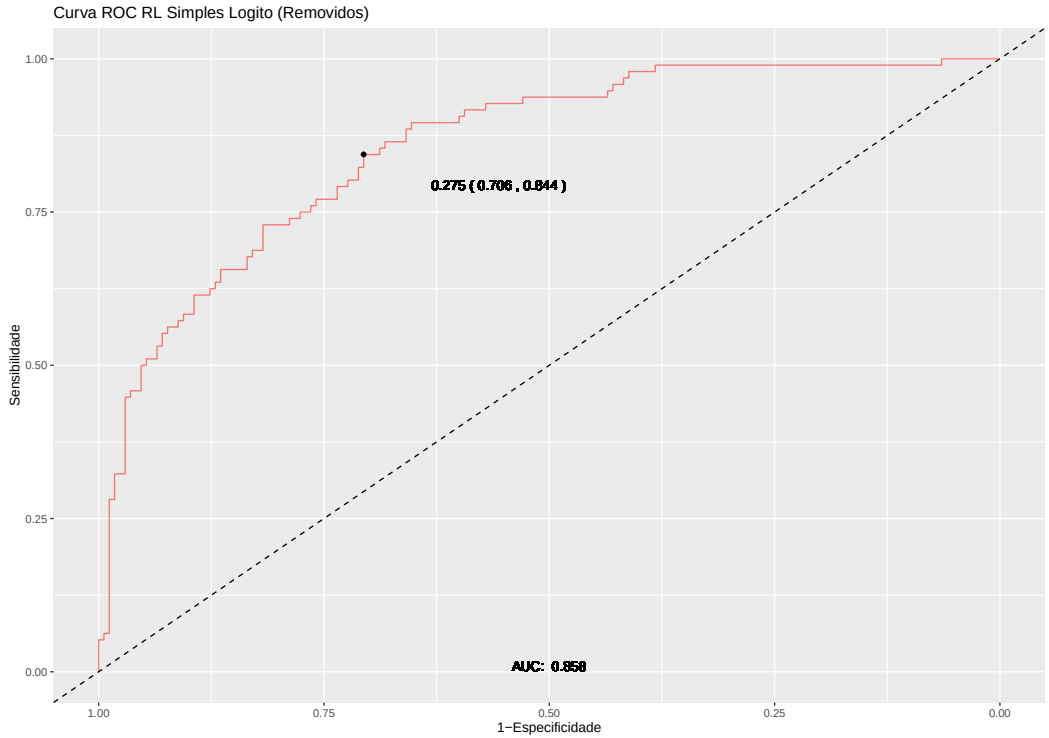


Desempenho do Modelo			
Accuracy	0.7764	**Sensitivity**	0.9167
95% CI	(0.7041, 0.8382)	**Specificity**	0.4906
No Information Rate	0.6708	**Pos Pred Value**	0.7857
P-Value [Acc >NIR]	0.002203	**Neg Pred Value**	0.7429
		Prevalence	0.6708
Kappa	0.4458	**Detection Rate**	0.6149
		Detection Prevalence	0.7826
Mcnemar's Test P-Value	0.004607	**Balanced Accuracy**	0.7036

Regressão Logística Simples (Partição 2)

	Referência	
Predito	**No**	**Yes**
No	64	11
Yes	4	10

- Validação cruzada ($k = 10$)
- Dados sem *missings*

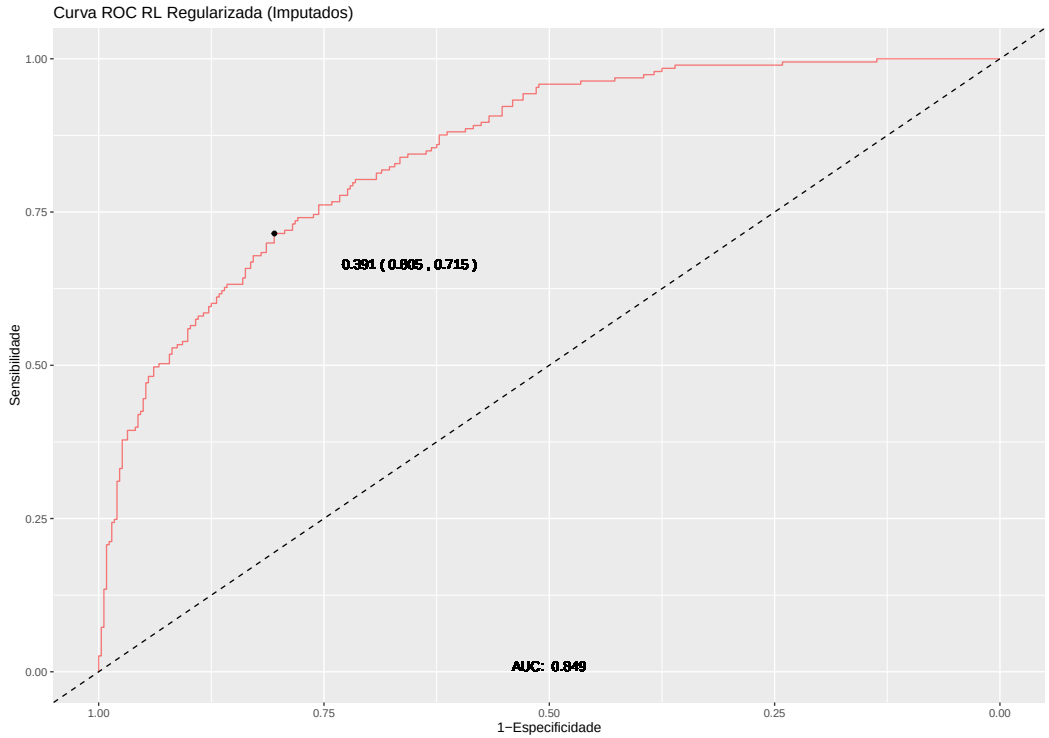


Desempenho do Modelo			
Accuracy	0.8315	**Sensitivity**	0.9412
95% CI	(0.7373, 0.9025)	**Specificity**	0.4762
No Information Rate	0.764	**Pos Pred Value**	0.8533
P-Value [Acc >NIR]	0.08127	**Neg Pred Value**	0.7143
		Prevalence	0.7640
Kappa	0.4717	**Detection Rate**	0.7191
		Detection Prevalence	0.8427
Mcnemar's Test P-Value	0.12134	**Balanced Accuracy**	0.7087

Regressão Logística Regularizada (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	99	28
Yes	9	25

- Validação cruzada ($k = 10$)
- Dados imputados

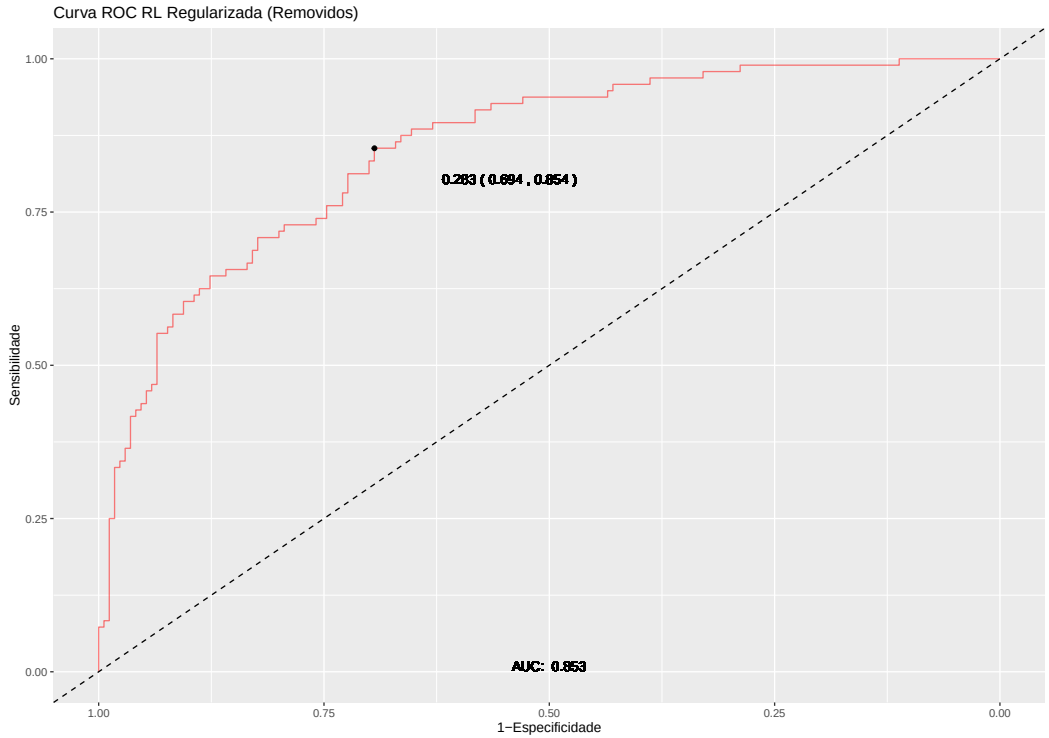


Desempenho do Modelo			
Accuracy	0.7702	**Sensitivity**	0.9167
95% CI	(0.6974, 0.8327)	**Specificity**	0.4717
No Information Rate	0.6708	**Pos Pred Value**	0.7795
P-Value [Acc >NIR]	0.003815	**Neg Pred Value**	0.7353
		Prevalence	0.6708
Kappa	0.4274	**Detection Rate**	0.6149
		Detection Prevalence	0.7888
Mcnemar's Test P-Value	0.003085	**Balanced Accuracy**	0.6942

Regressão Logística Regularizada (Partição 2)

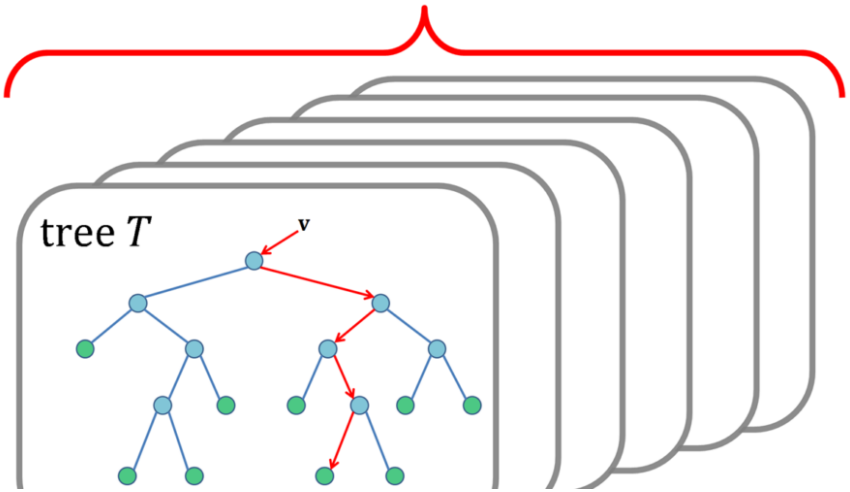
	Referência	
Predito	**No**	**Yes**
No	64	11
Yes	4	10

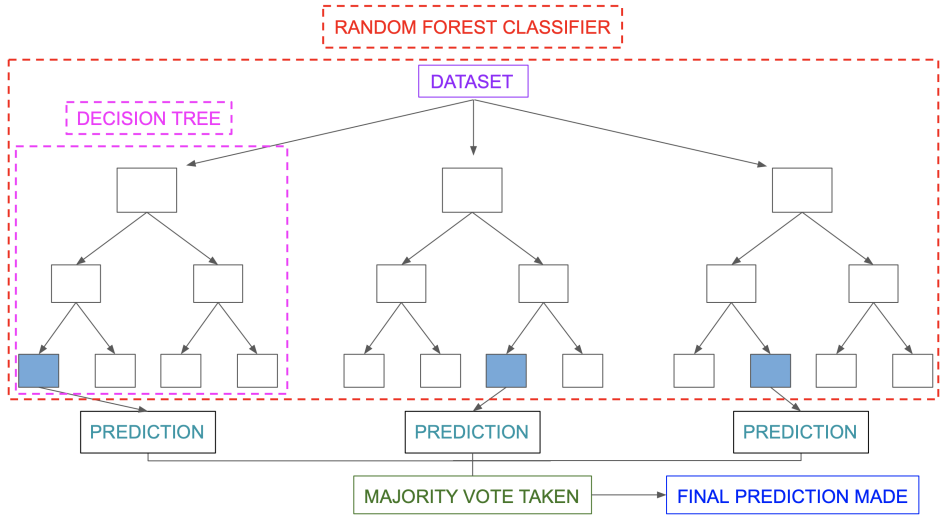
- Validação cruzada ($k = 10$)
- Dados sem *missings*



Desempenho do Modelo			
Accuracy	0.8315	**Sensitivity**	0.9412
95% CI	(0.7373, 0.9025)	**Specificity**	0.4762
No Information Rate	0.764	**Pos Pred Value**	0.8533
P-Value [Acc >NIR]	0.08127	**Neg Pred Value**	0.7143
		Prevalence	0.7640
Kappa	0.4717	**Detection Rate**	0.7191
		Detection Prevalence	0.8427
Mcnemar's Test P-Value	0.12134	**Balanced Accuracy**	0.7087

Random Forest

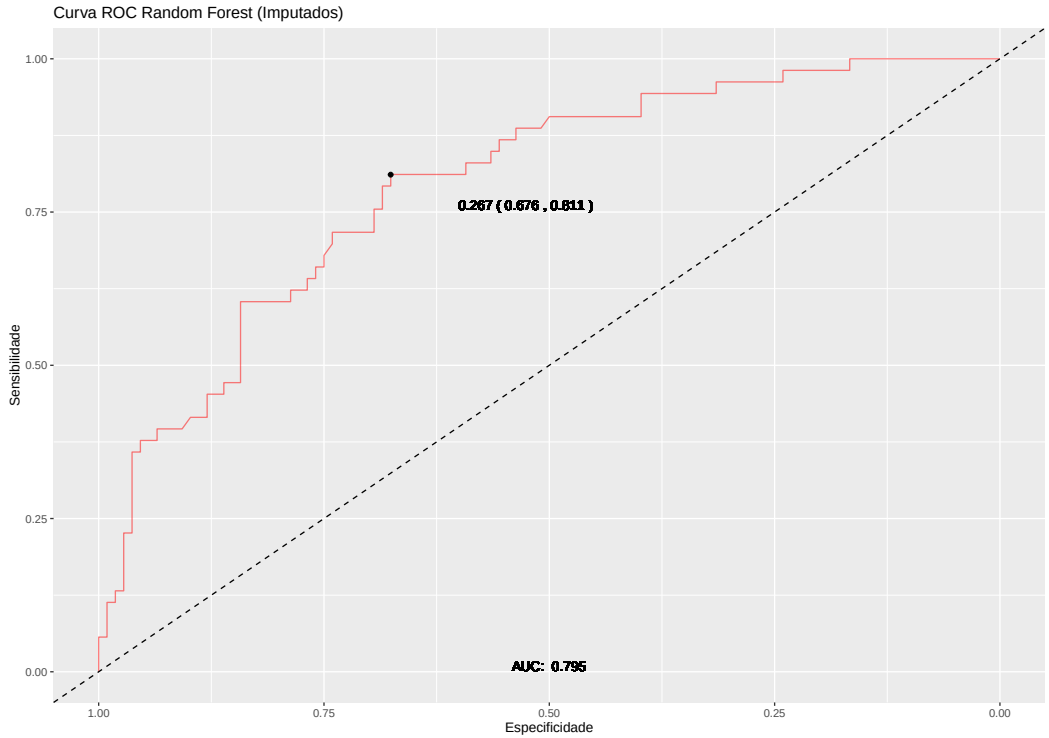




Random Forest (Partição 1)

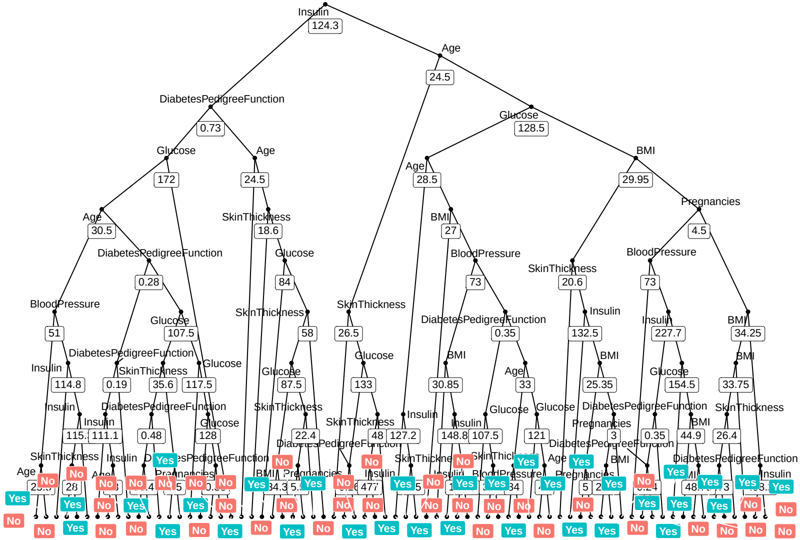
	Referência	
Predito	**No**	**Yes**
No	93	28
Yes	15	25

- Validação cruzada ($k = 10$)
- Dados imputados



Desempenho do Modelo			
Accuracy	0.7329	Sensitivity	0.8611
95% CI	(0.6576, 0.7995)	Specificity	0.4717
No Information Rate	0.6708	Pos Pred Value	0.7686
P-Value [Acc >NIR]	0.05368	Neg Pred Value	0.6250
		Prevalence	0.6708
Kappa	0.355	Detection Rate	0.5776
		Detection Prevalence	0.7516
Mcnemar's Test P-Value	0.06725	Balanced Accuracy	0.6664

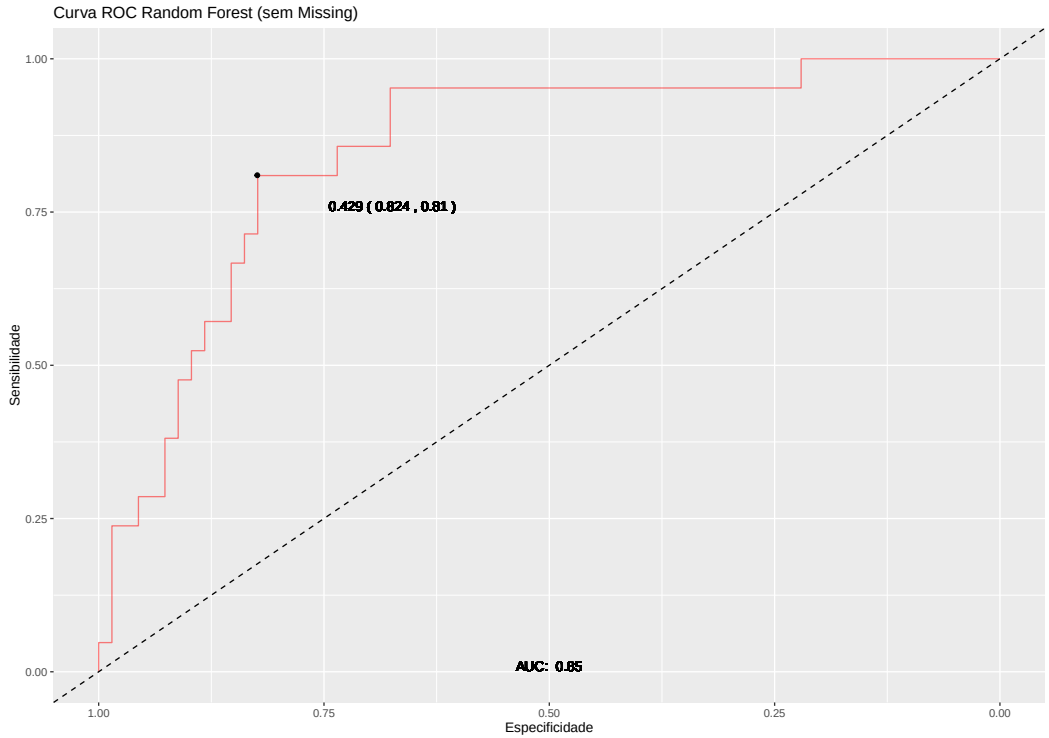
Partição 1: Menor árvore com imputação 250



Random Forest (Partição 2)

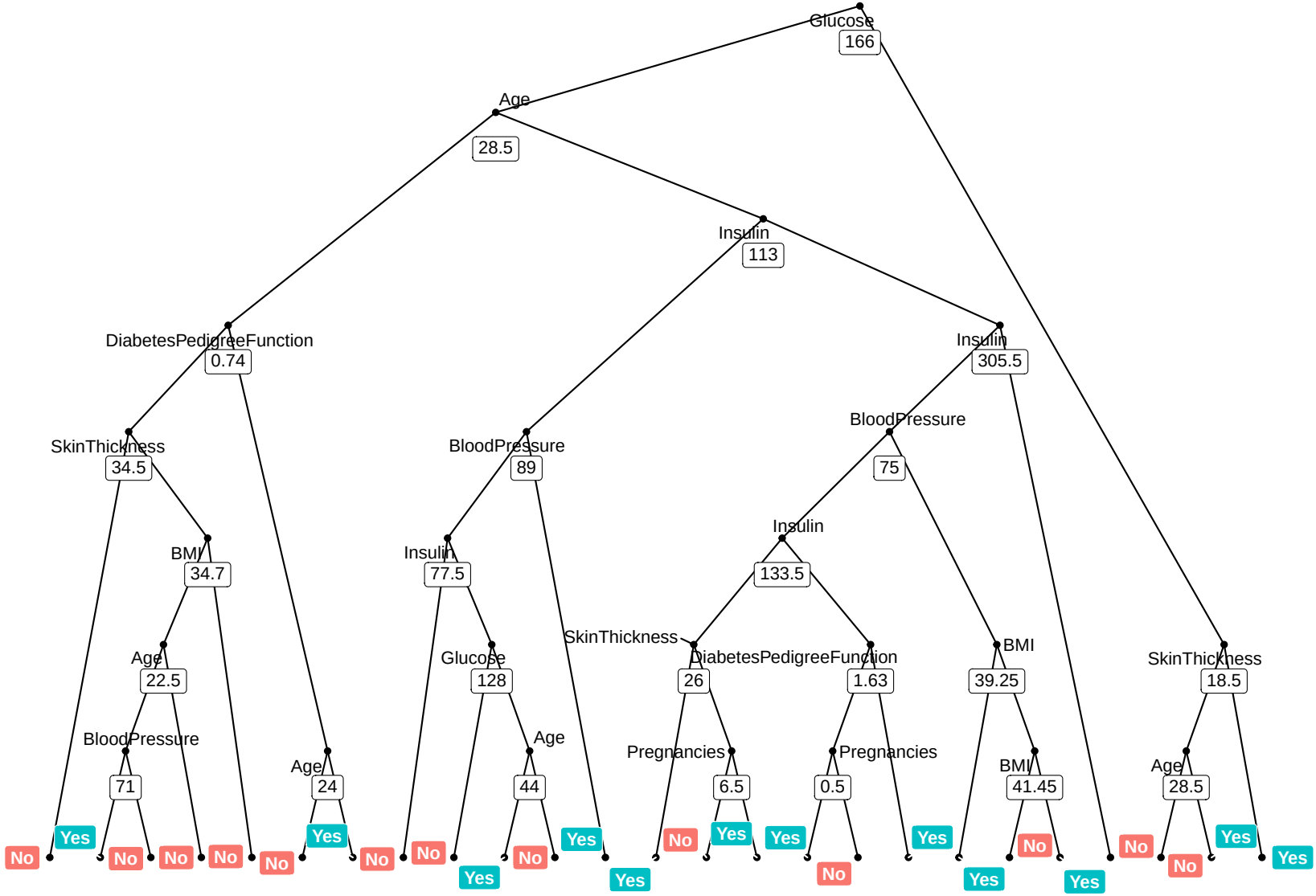
	Referência	
Predito	**No**	**Yes**
No	59	9
Yes	9	12

- Validação cruzada ($k = 10$)
- Dados sem *missings*

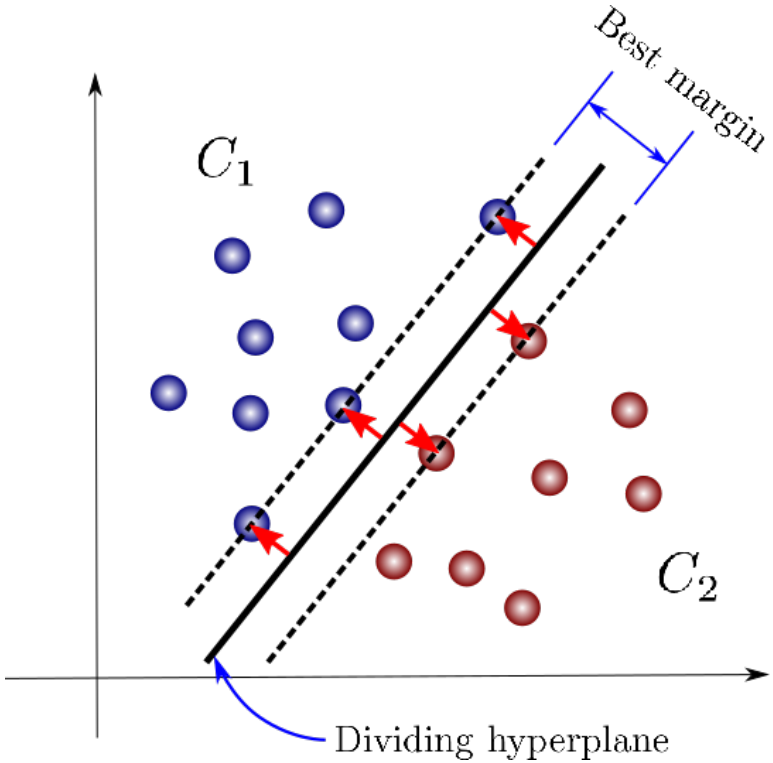


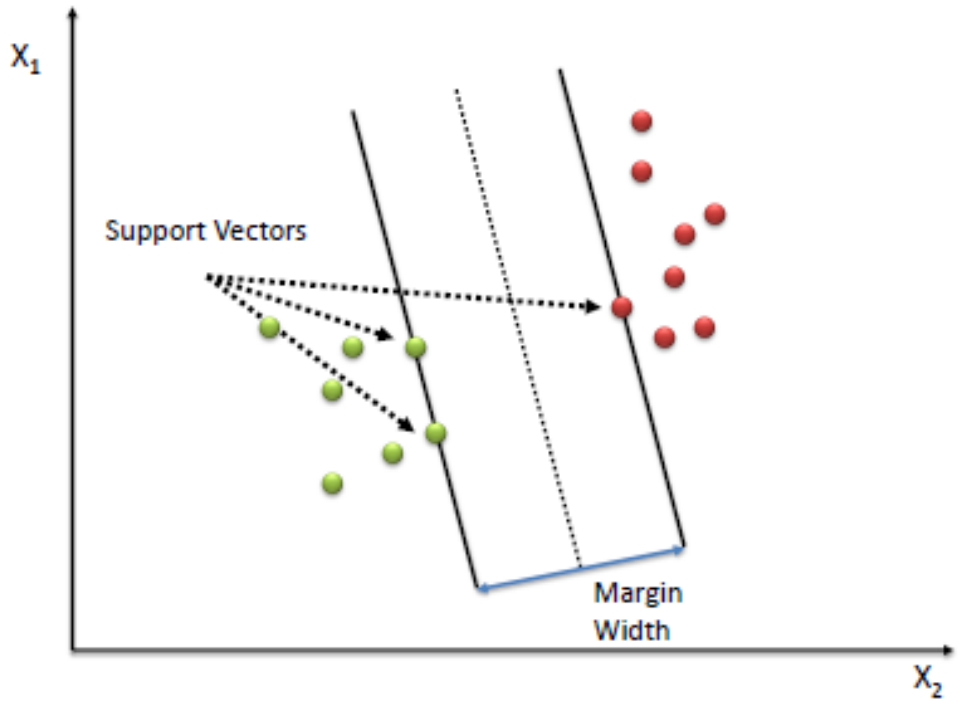
Desempenho do Modelo			
Accuracy	0.7978	Sensitivity	0.8676
95% CI	(0.6993, 0.8755)	Specificity	0.5714
No Information Rate	0.764	Pos Pred Value	0.8676
P-Value [Acc >NIR]	0.2709	Neg Pred Value	0.5714
		Prevalence	0.7640
Kappa	0.4391	Detection Rate	0.6629
		Detection Prevalence	0.7640
Mcnemar's Test P-Value	1.0000	Balanced Accuracy	0.7195

Partição 2: Menor árvore sem imputação: 250



Support Vector Machine

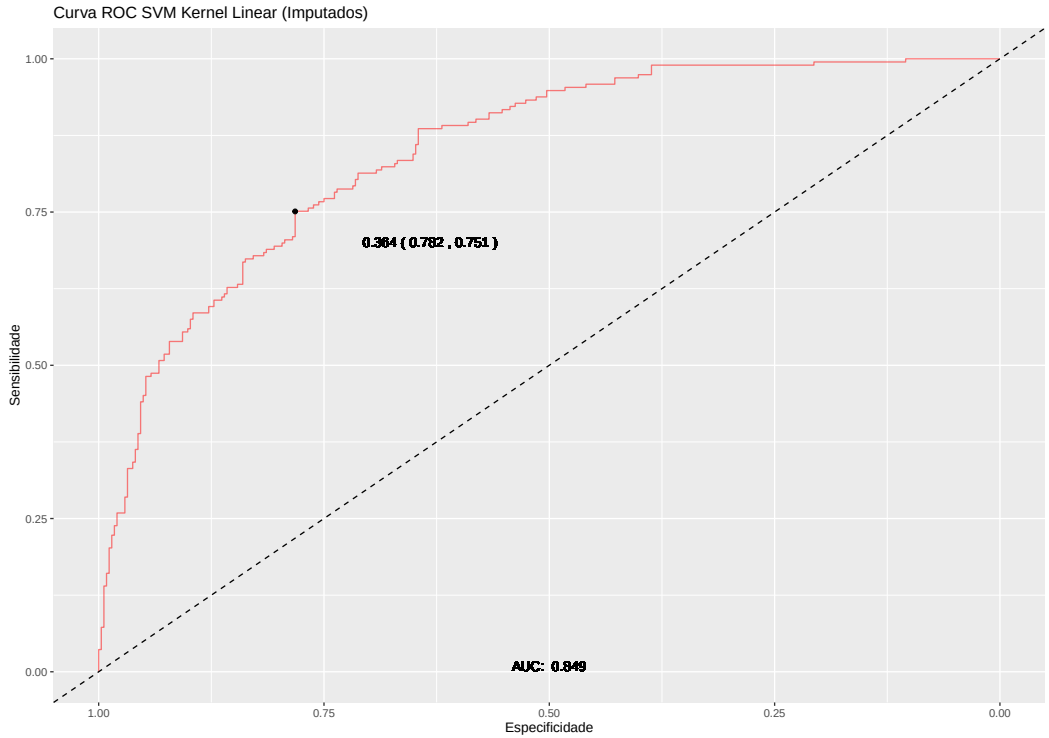




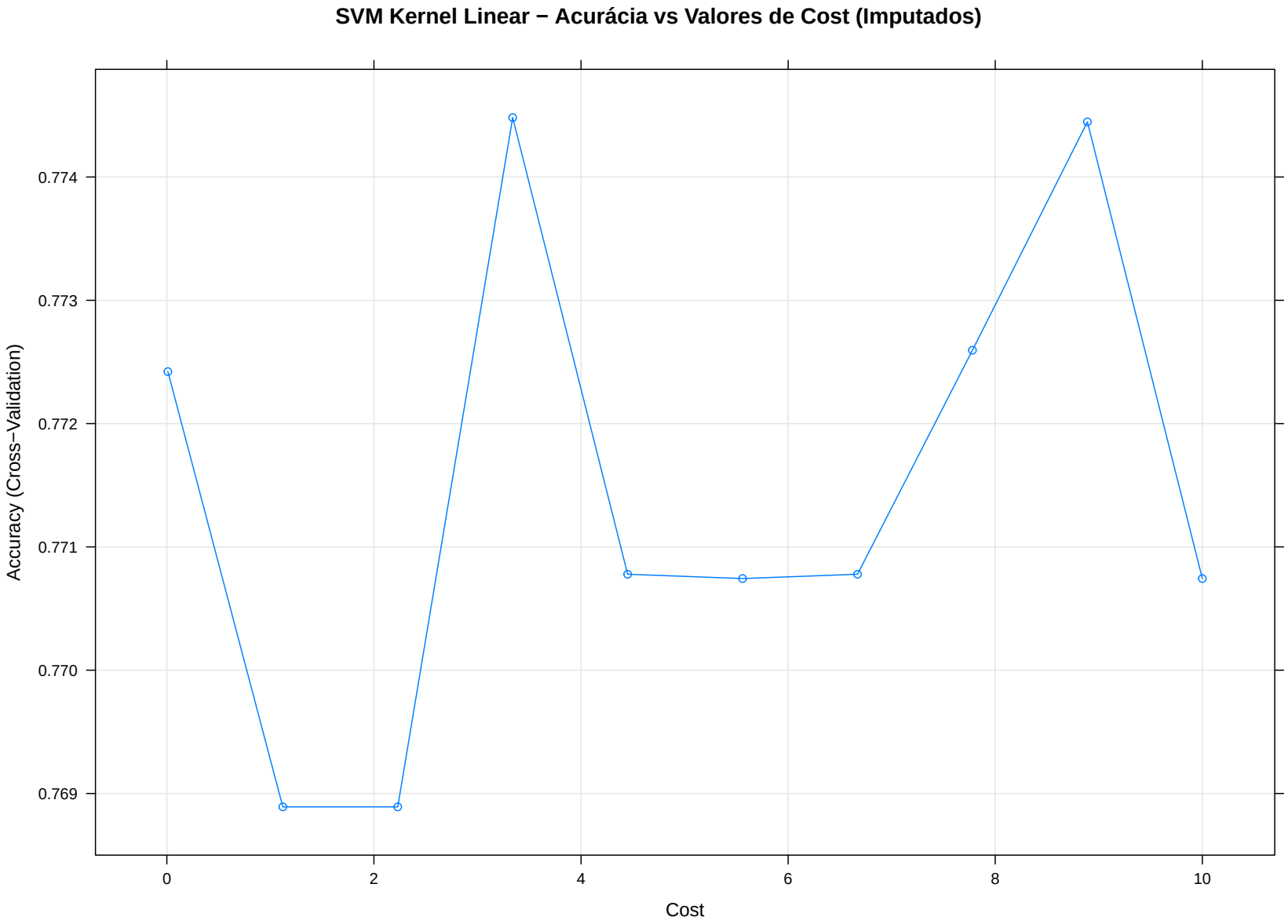
SVM *Kernel* Linear (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	98	27
Yes	10	26

- Validação cruzada ($k = 10$)
- Dados imputados



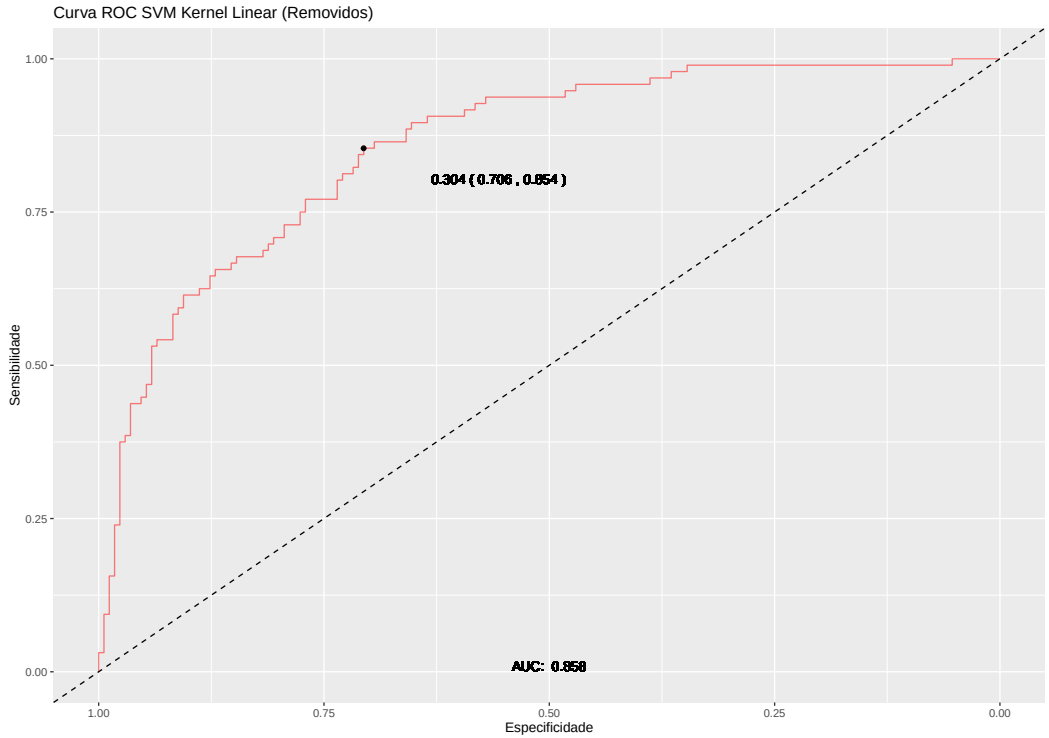
Desempenho do Modelo			
Accuracy	0.7702	Sensitivity	0.9074
95% CI	(0.6974, 0.8327)	Specificity	0.4906
No Information Rate	0.6708	Pos Pred Value	0.7840
P-Value [Acc >NIR]	0.003815	Neg Pred Value	0.7222
		Prevalence	0.6708
Kappa	0.4334	Detection Rate	0.6087
		Detection Prevalence	0.7764
Mcnemar's Test P-Value	0.008529	Balanced Accuracy	0.6990


SVM Kernel Linear − Acurácia vs Valores de Cost (Imputados)
Accuracy (Cross−Validation)
0.774
0.773
0.772
0.771
0.770
0.769
0
2
4
6
8
10
Cost

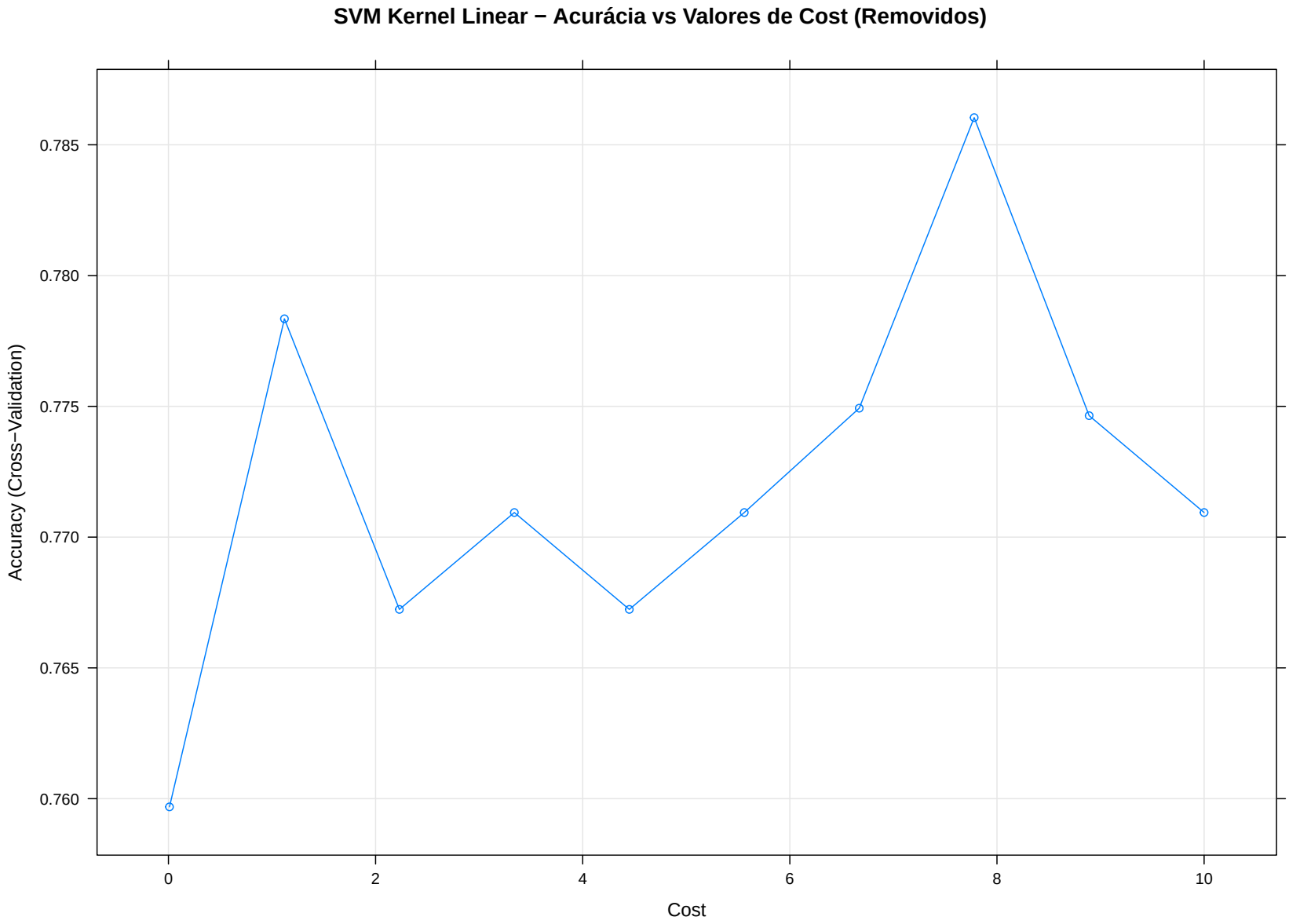
SVM *Kernel* Linear (Partição 2)

	Referência	
Predito	**No**	**Yes**
No	64	12
Yes	4	9

- Validação cruzada ($k = 10$)
- Dados sem *missings*



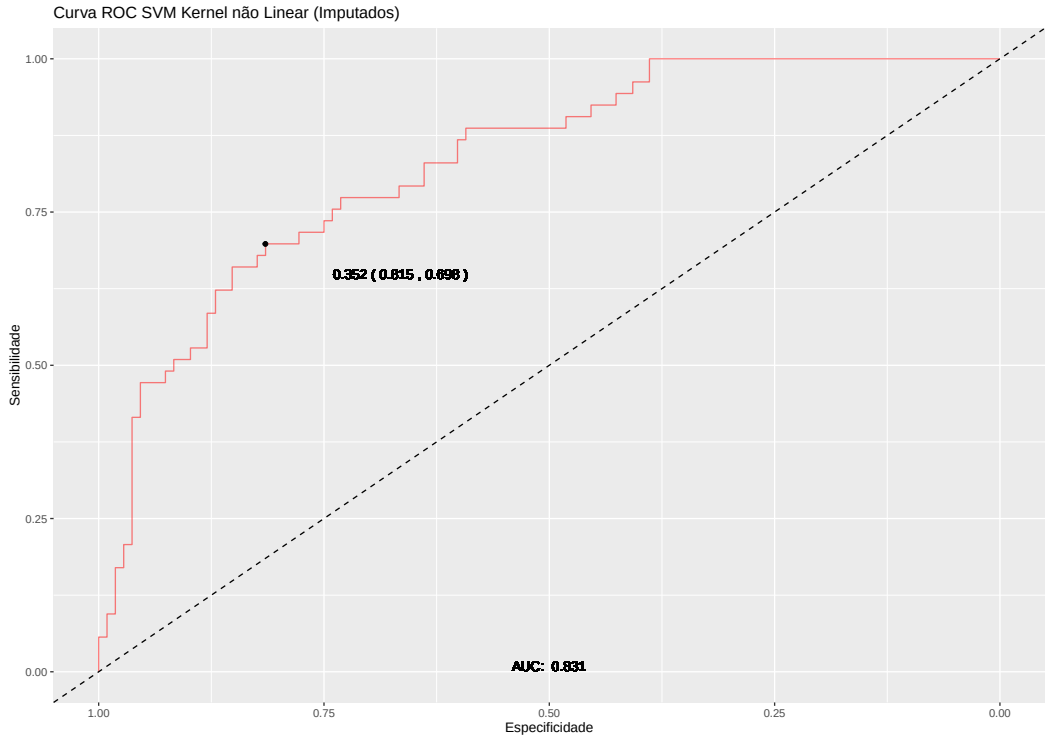
Desempenho do Modelo			
Accuracy	0.8202	Sensitivity	0.9412
95% CI	(0.7245, 0.8936)	Specificity	0.4286
No Information Rate	0.764	Pos Pred Value	0.8421
P-Value [Acc >NIR]	0.12910	Neg Pred Value	0.6923
		Prevalence	0.7640
Kappa	0.4258	Detection Rate	0.7191
		Detection Prevalence	0.8539
Mcnemar's Test P-Value	0.08012	Balanced Accuracy	0.6849


SVM Kernel Linear − Acurácia vs Valores de Cost (Removidos)
Accuracy (Cross−Validation)
0.760
0.765
0.770
0.775
0.780
0.785
0
2
4
6
8
10
Cost

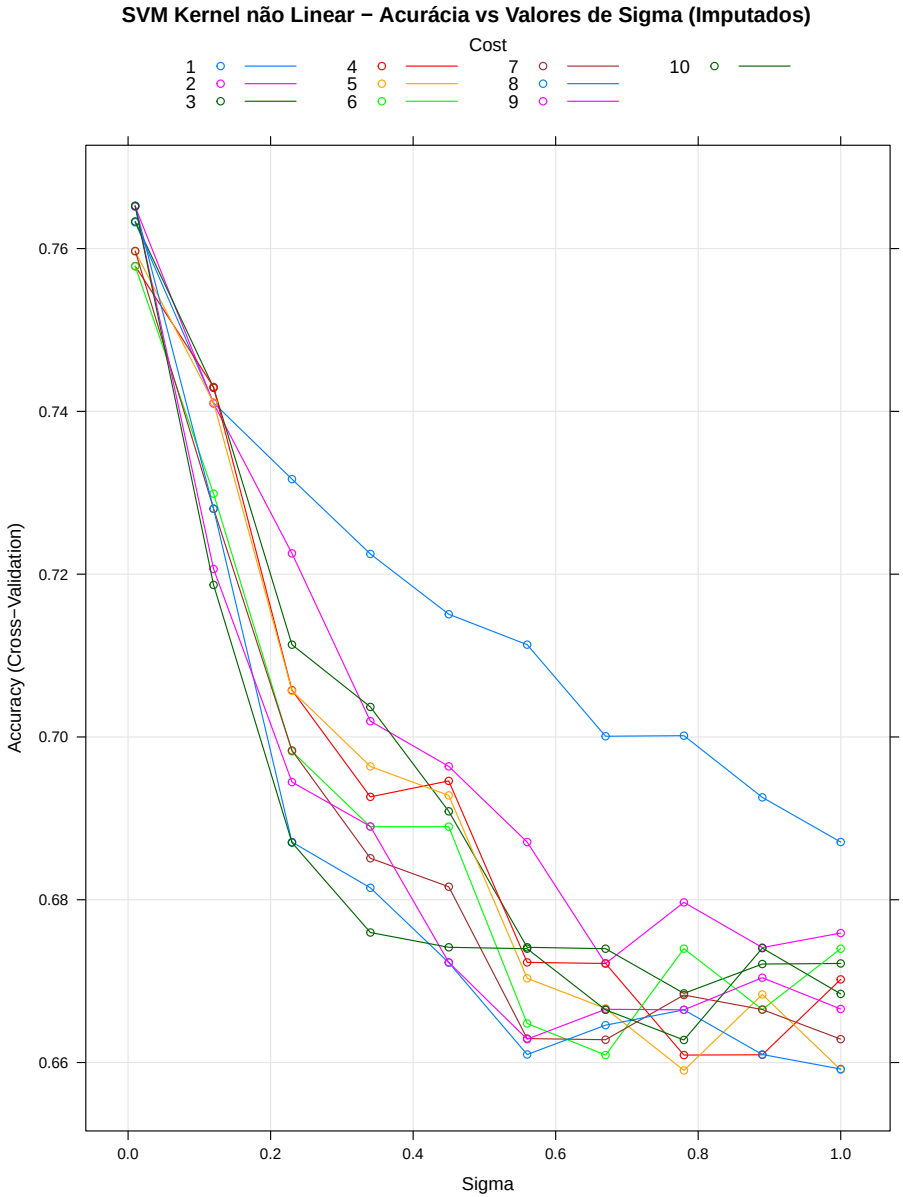
SVM *Kernel* Não-Linear (Partição 1)

	Referência	
Predito	**No**	**Yes**
No	99	26
Yes	9	27

- Validação cruzada ($k = 10$)
- Dados imputados



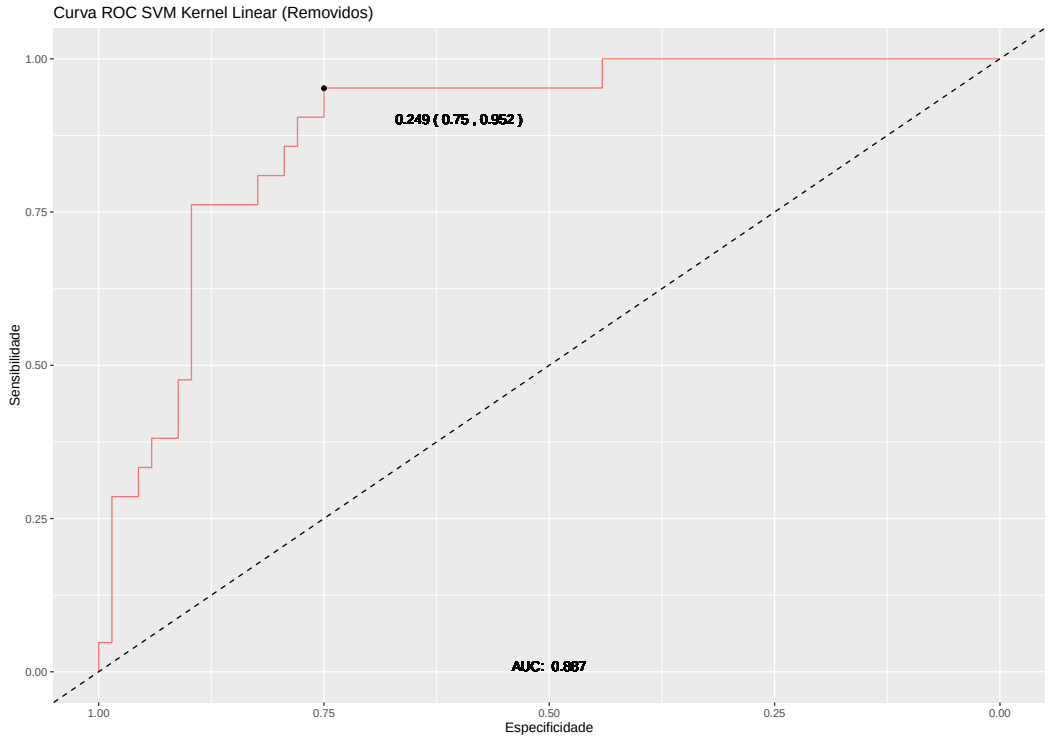
Desempenho do Modelo			
Accuracy	0.7826	Sensitivity	0.9167
95% CI	(0.7109, 0.8437)	Specificity	0.5094
No Information Rate	0.6708	Pos Pred Value	0.7920
P-Value [Acc >NIR]	0.001230	Neg Pred Value	0.7500
		Prevalence	0.6708
Kappa	0.464	Detection Rate	0.6149
		Detection Prevalence	0.7764
Mcnemar's Test P-Value	0.006841	Balanced Accuracy	0.7131


SVM Kernel não Linear − Acurácia vs Valores de Sigma (Imputados)
Cost
1
2
3
4
5
6
7
8
9
10
Accuracy (Cross−Validation)
0.66
0.68
0.70
0.72
0.74
0.76
Sigma
0.0
0.2
0.4
0.6
0.8
1.0

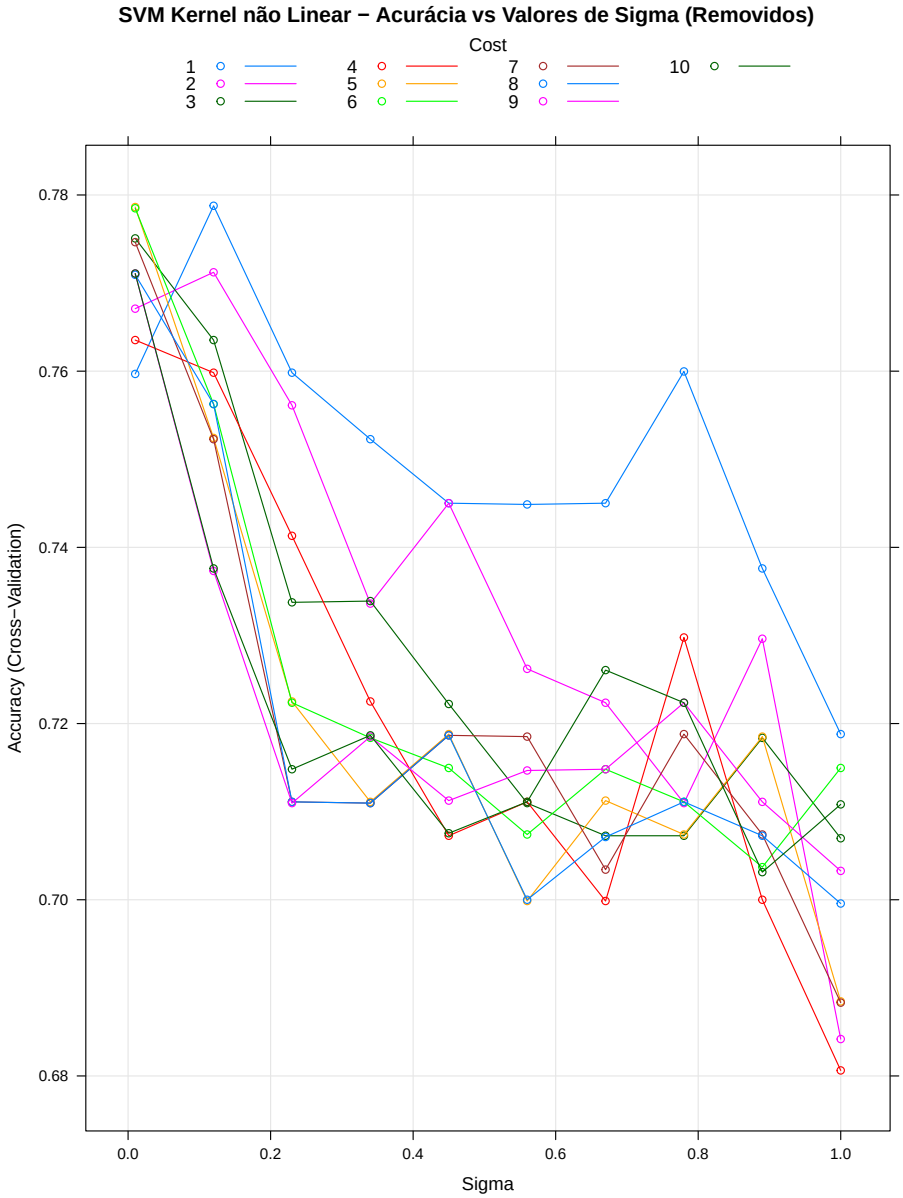
SVM *Kernel* Não-Linear (Partição 2)

	Referência	
Predito	**No**	**Yes**
No	63	13
Yes	5	8

- Validação cruzada ($k = 10$)
- Dados sem *missings*



Desempenho do Modelo			
Accuracy	0.7978	Sensitivity	0.9265
95% CI	(0.6993, 0.8755)	Specificity	0.3810
No Information Rate	0.764	Pos Pred Value	0.8289
P-Value [Acc >NIR]	0.27088	Neg Pred Value	0.6154
		Prevalence	0.7640
Kappa	0.354	Detection Rate	0.7079
		Detection Prevalence	0.8539
Mcnemar's Test P-Value	0.09896	Balanced Accuracy	0.6537


SVM Kernel não Linear − Acurácia vs Valores de Sigma (Removidos)
Cost
1
2
3
4
5
6
7
8
9
10
Accuracy (Cross−Validation)
0.78
0.76
0.74
0.72
0.70
0.68
0.0
0.2
0.4
0.6
0.8
1.0
Sigma

Comparação dos Modelos

Métricas: Acurácia, Sensibilidade, Especificidade e Acurácia Balanceada

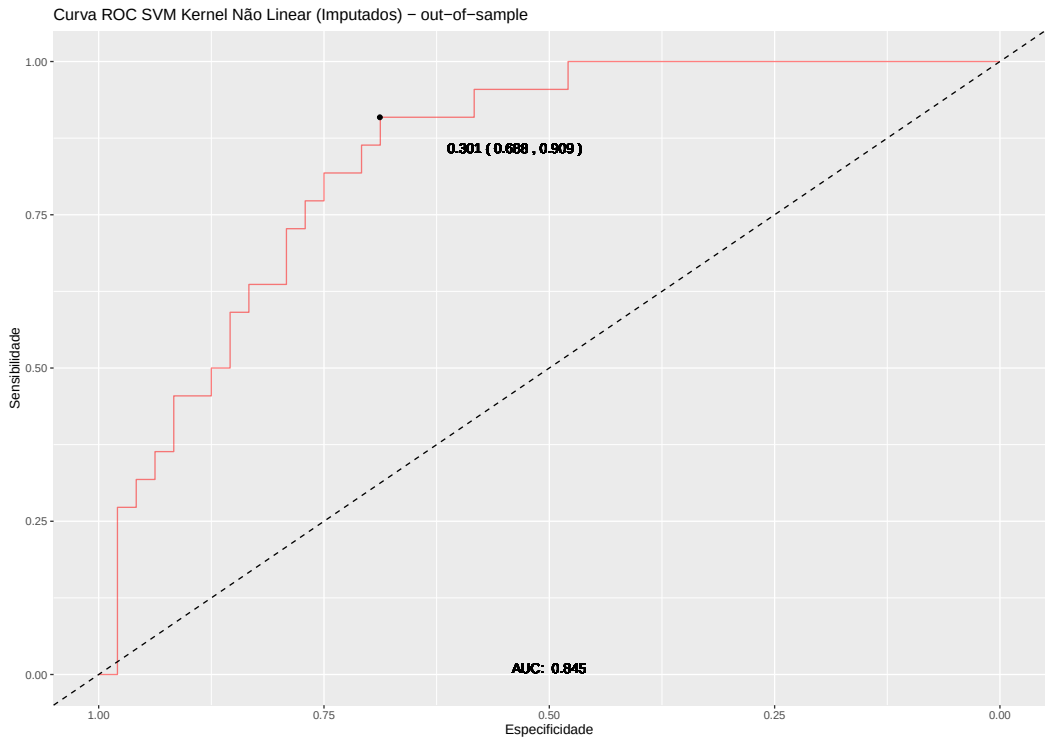
Modelo	Imputados				Removidos			
	Acuracia	Sensibilidade	Especificidade	Acurácia Balanceada	Acurácia	Sensibilidade	Especificidade	Acurácia Balanceada
AD Linear	0.77	0.91	0.47	0.69	0.82	0.94	0.42	0.68
AD Flexível	0.75	0.87	0.50	0.69	0.79	0.89	0.47	0.68
AD Quadrática	0.77	0.88	0.52	0.70	0.84	0.88	0.71	0.79
RL Simples	0.77	0.91	0.49	0.70	0.83	0.94	0.47	0.7
RL Regularizada	0.77	0.91	0.47	0.69	0.83	0.94	0.47	0.7
Random Forest	0.73	0.86	0.47	0.66	0.79	0.86	0.57	0.71
SVM Linear	0.77	0.9	0.49	0.69	0.82	0.94	0.42	0.68
SVM Ñ Linear	0.78	0.91	0.50	0.71	0.79	0.92	0.38	0.65

SVM *Kernel* Não-Linear (Partição 1)

Teste: Desempenho sobre *out-of-sample*

	Referência	
Predito	**No**	**Yes**
No	38	8
Yes	10	14

- Validação cruzada ($k = 10$)
- Dados imputados



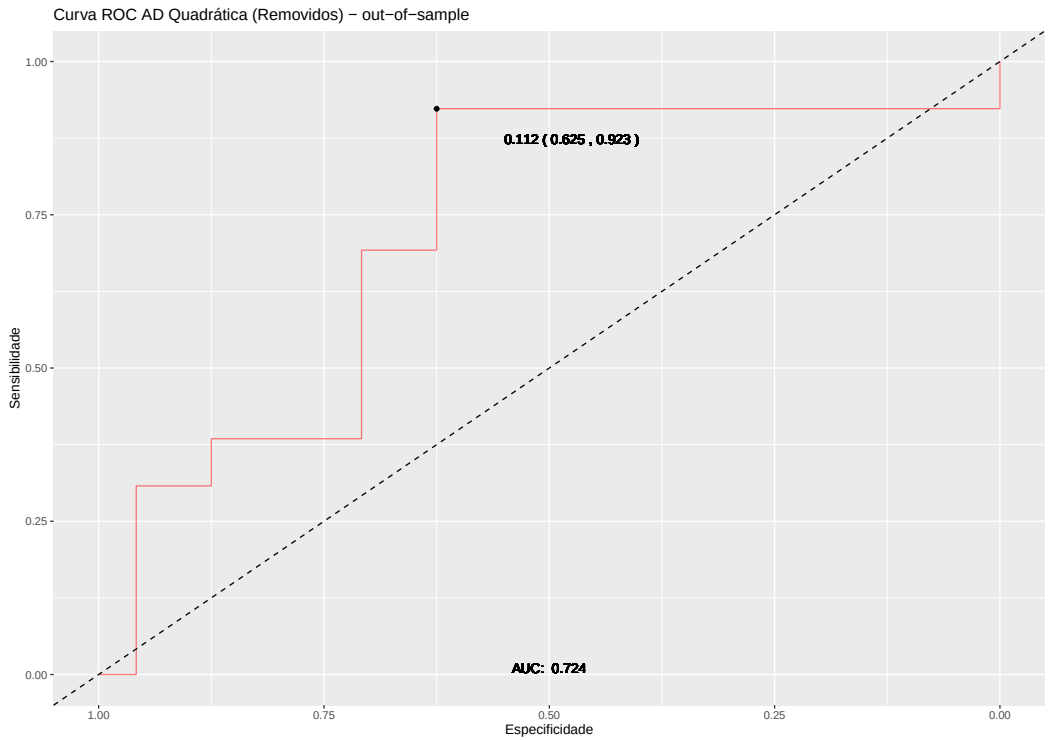
Desempenho do Modelo			
Accuracy	0.7429	Sensitivity	0.7917
95% CI	(0.6244, 0.8399)	Specificity	0.6364
No Information Rate	0.6857	Pos Pred Value	0.8261
P-Value [Acc >NIR]	0.1846	Neg Pred Value	0.5833
		Prevalence	0.6857
Kappa	0.4177	Detection Rate	0.5429
		Detection Prevalence	0.6571
Mcnemar's Test P-Value	0.8137	Balanced Accuracy	0.7140

Análise Discriminante Quadrática (Partição 2)

Teste: Desempenho sobre *out-of-sample*

	Referência	
Predito	**No**	**Yes**
No	17	5
Yes	7	8

- Validação cruzada ($k = 10$)
- Dados sem *missings*



Desempenho do Modelo			
Accuracy	0.6757	Sensitivity	0.7083
95% CI	(0.5021, 0.8199)	Specificity	0.6154
No Information Rate	0.6486	Pos Pred Value	0.7727
P-Value [Acc >NIR]	0.4384	Neg Pred Value	0.5333
		Prevalence	0.6486
Kappa	0.3127	Detection Rate	0.4595
		Detection Prevalence	0.5946
Mcnemar's Test P-Value	0.7728	Balanced Accuracy	0.6619

Outras implementações...

Dúvidas, comentários ou sugestões?

Envie-nos um e-mail

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- vitorhugo@usp.br

Referências:

Smith, J.W., Everhart, J.E., Dickson, W.C., Knowler, W.C., & Johannes, R.S. (1988). *Using the ADAP Learning Algorithm to Forecast the Onset of Diabetes Mellitus.* In: Proceedings of the Symposium on Computer Applications and Medical Care (pp. 261–265). IEEE Computer Society Press.

Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani (2014). *An Introduction to Statistical Learning: with Applications in R.* Springer New York.

Trevor Hastie, Robert Tibshirani, Jerome Friedman (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction.* 2 ed. Springer New York.